Cineca HPC Report

2014

High Performance Computing Infrastructure

High Performance Data Analytics

Community Code Activities

Solutions for Innovation

Data Management

Cloud Computing

problem solving

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Cineca HPC Report

Dear Colleague,

This second edition of the Cineca HPC Annual Report continues our commitment to offer data and information about our effort and impact in High Performance Computing on the scientific community and to share with all our stakeholders our vision and perspectives of development. In this 2014 report we go on in providing an overall panorama of our activities and of the research outcomes obtained by means of the access to our supercomputing infrastructure both at national and at European level; at the same time we provide an assessment about our intangible assets which, beyond the metric of the consolidated indexes of performance, represents the goodwill value of our mission.

2014 has been a dense and a crucial year for us.
The introduction of a petascale class Tier-1 supercomputing system, results of a joint economical effort of Cineca, National Institute of High Energy Physics (INFN) and some other qualified national partners, including some Universities, Members of the Cineca Consortium, represents a profitable development model for further opportunities in the future.
The installation of PICO, the Big Data system, which enables new Big Data classes of applications, related to the management and processing of large volume of data, coming from both simulations and experiments and the particular focus on all emerging scenarios which require an interactive model (Urgent Computing), as well as new paradigms of resource utilization through Cloud Computing technology have been our daily focus during the last months.

The set up of the procedure for the replacement of our Tier-0, Fermi, opens the door for us to a new challenging year, for which our objective will be that the scientific community is allowed to continue to take full advantage of the new computing architectures and platforms that we will provide.

High quality based on qualified expertise, development of knowledge, original solutions have formed and will be the basis of our position of national point of reference for a digital infrastructure of international relevance for high performance intensive and throughput computing and high performance data processing and analytics.

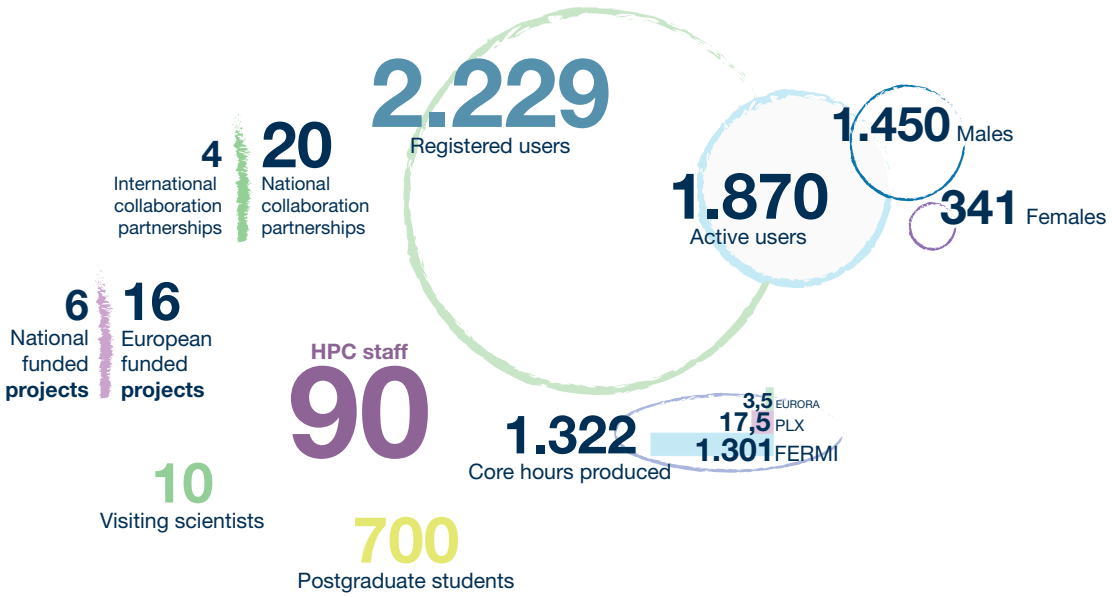
Sanzio Bassini

Director of SuperComputing Applications and Innovation Department of Cineca

Identity, Values and Mission

Cineca is a non profit Consortium, made up of 69 Universities and 3 Research Institutes, plus the Ministry of University and Research, and today is the largest Italian supercomputing centre. With more than seven hundred employees, it operates in the technological transfer sector through High Performance Computing and High Performance Data Analytics, management and development of networks and web-based services, and development of complex information systems for treating large amounts of data. Today Cineca is the high-technology bridge between the academic and research world, and the world of industry and public administration.
The department in charge of HPC and HPDA is SCAI, SuperComputing Applications and Innovation Department, led by Sanzio Bassini.
Starting from 1969, when the Ministry of Education supported four universities in the idea of consortiating and creating a supercomputing centre in Bologna with the CDC 6600, the first system designed by Seymour Cray, today, after the merging of the three Italian consortia Cineca, Cilea and Caspur, Cineca is a unique national consortium (of multiple sites, Bologna, Rome and Milan) with the major aim of supporting Italian research.
For 45 years, Cineca and its HPC department have been leaders in Italy in the deployment of a solid and trustable HPC environment, being the reference point for the national academic and research system, conveying the most advanced technical and scientific expertise in its young and multi-disciplinary staff, offering rich experience, highly flexible support, and customizable services to assist its national and European users.

Certifications
The Quality Management System of Cineca is compliant with the international standard ISO 9001, since November 2001.
The Information Security Management System of Cineca is compliant with the international standard ISO 27001 since 2005 (ex. BS 7799).



SECTION 1

ONE YEAR OF HPC AT CINECA

2014 in a nutshell

To create development and make it shareable by as many people as possible, in a European and world-wide panorama that is complex and in constant motion and evolution. To place the researcher and the frontier of science at the centre of every action and choice, both at technological and organizational level.

These are the two goals that the HPC team at Cineca chose to face, such as THE challenges of 2014, towards a future which promises to be of great changes in the world of research and of the research infrastructures, at least in Europe.

Deep transformations, such as new strategies, new and wider collaborations, new projects and a new internal organization led SCAI, the HPC department of Cineca, to a more focalized, somehow selective, so more effective action towards our stakeholders at large, and our users first.

The collaboration with institutions and research institutes of the highest value at the European level has made the SCAI activities across the border of paramount importance.

The scientific and technical experts of the department were undoubtedly the champions of the relevant achievements reached in last year. Their knowledge and expertise made them become the real protagonists of the big game of supporting the best science by promoting the best technologies and methodologies.

Special attention has been dedicated to training as an important mission at the service of the scientific communities (for the Italian ones through dedicated HPC national schools and courses and for the international ones through hosting and managing one of the six PRACE Advanced Training Centres) and to training of the staff as well, to offer more and more instruments for them to play every day at the forefront and acting as a driving force, offering a trustable and proactive technological presence in a huge number of important scientific challenges of our users.

Our strategic goals:

- day-by-day activity driven by the potential to improve the best science of our users;
- work in connection with our stakeholders to achieve and widen an integrated national system for the support of science at large;
- build capacity and excellence in our human resources, our most valuable asset.

Technology is a key enabler for any organization and becomes THE mission for an institution acting as national centre for HPC, HPDA and support to science. Major improvements have been made to the infrastructure during the past year: Fermi, the flagship system Blue Gene/Q, has been joined by a new computing system, PICO, that aims at responding to the ever-growing demand of services and capacities (storage, management, compute, and visualization) which are essential to address the challenge of "big data" problems, nowadays a key factor of many scientific disciplines. PICO is devoted to data intensive computing cases and features peculiar hardware characteristics (e.g. SSD storage), software tools, and the high-throughput techniques needed by data-driven projects. The objective is to provide users with the instruments required to address all the challenges that arise when either the volume of data, their internal structure, or the velocity at which they are collected make them difficult to be processed and managed. The second big new entry is a system, at the time of this report in installation phase, with 1Pf performance that will serve the Italian community, as Tier-1, representing possibly in nuce the starting step for the replacement of the Tier-0 during 2015 as from the Cineca roadmap recently published.

The provision of world class infrastructure and world class research support will enable our researchers to conduct high quality research and us to continue in our mission of attract and support research talents.

In the next couple of years it is our convicement that the supercomputing centres, as large scale facilities, will have to lead a process to move towards the creation of a digital infrastructure on top of the geographical data transport network, or in other words the research networks, GARR at national level, GEANT at European level. Such a digital infrastructure layer would have to combine and interoperate Supercomputing resources for high performance intensive computing, throughput computing, data processing computing and data management for long term curation and preservation. This process began to progress by means of the agreement between INFN and Cineca for a joint development action, which created the condition for a joint economical effort between the two entities to fund the procurement of the Tier-1 system which is currently under installation at Cineca premises. This first step may open a new paradigm for the development of computational science in Italy, and may potentially represent a model at European level.

Cineca will work and collaborate with INFN in order to create in Italy a structured persistent and competitive at world-class level digital infrastructure, opening to the whole Italian scientific community an integrated environment covering HPC, HPTC, HPDA allowing a significant breakthrough in the management of research data.

Sanzio Bassini, Francesca Garofalo
Cineca


PRACE Tier-0
FERMI - IBM BG/Q
10K computing nodes
160K cores
2 PFlop/s Peak Performance
National Tier-1
IBM NeXtScale Cluster
512 nodes, Intel Haswell
8K cores
768 accelerators (Intel Xeon Phi)
High Performance Data Analytics
PICO - IBM NeXtScale Cluster
80 computing nodes
• structured and unstructured data processing
• hadoop and map reduce
• data insight
• remote visualization
• cloud computing
Data repository, curation and preservation
Multi tier storage
40 TB fast (SSD) storage
5 PB GSS storage
12 PB TAPE storage, integrated with GSS through LTFS
SISSA - ISAS
International School for Advanced Studies
ELETTRA SINCROTRONE
ICTP
International Centre for Theoretical Physics
OGS
National Institute of Oceanography and Experimental Geophysics
CINECA
IIT
The Italian Institute of Technology
RER
Emilia Romagna Region
LENS
European Laboratory for Non-linear Spectroscopy
CNR
National Research Council
INAF - IASF
National Institute of Astrophysics
Civil Protection
INFN
National Institute of Nuclear Physics
CMCC
Euro-Mediterranean Center on Climate Change

2014 systems upgrade

The year 2014 started for the HPC in Cineca with the procurement of new hardware.
What is it all about?
Part of the new hardware infrastructure makes available a fairly large amount of storage composed of 4 PetaByte of disk space and 12 PetaByte of tape space. It is possible to say that Big Data in Cineca is now a real opportunity, not only a fashionable Information Technology's word. The capacity of this storage infrastructure isn't the only interesting characteristic. Fast access and a special software feature that moves automatically data from disk space to tapes, depending on the age and the dimensions of the data, are valuable charcateristics.
These multiple levels of data access best fit the performance and capacity requirements of different applications. The new infrastructure makes available tens of processing nodes for the data management and for different use of data like running data analytics software (open and legacy), data post processing, remote visualization and operating system virtualization.
In addition to the above system, a new cluster for the technical computing has been procured.
The IBM Dataplex PLX has been replaced by an IBM Nextscale system equipped with the Intel Haswell processors and graphic Xeon Phi accelerators providing a huge increase in performance.
The computational capacity of the new cluster is 1 PFlops. The system will be the national Tier-1 machine for hosting industrial applications for innovations, weather forecasts, ISCRA scientific projects, as its predecessor.
Aside the new entries the legacy infrastructure is still providing full services.
FERMI, the IBM Blue Gene/Q system continues to deliver hundreds of million of cpu hours for the researchers whose projects have been awarded resources by the PRACE and the ISCRA selection. The Blue Gene/Q was still the number 17 of the last June top 500 list of the most powerful supercomputers of the world.
EURORA, the Eurotech prototype procured within the PRACE implementation project, is now in its phase-out.
Looking at the future and at the next decade, we may foresee that in a couple of further technological steps the exascale performance could be reached around year 2020.
From the environment point of view, a thorough analysis and a deep revision of the machine room power consumption and cooling have been carried out. Cineca, in collaboration with the University of Bologna, simulated different environment scenarios for different cooling method. The outcome is the revamp of all the Power Supply System Units and the increase of the number of chiller machines that work in free cooling mode.
The availability and use of large datasets in many scientific fields represents at the same time new opportunities but also new challenges. Often referred to as a data deluge, massive datasets is not only revolutionizing the way research is carried out but results in the emergence of reconceptualizing computational and data resources to afford data-intensive applications in their various forms. Data-dominated science necessitates of a new way of designing, organizing and operating infrastructure to respond to this revolution. In order to allow the users to fully exploit accumulated data and knowledge, a new approach in the design of the Cineca infrastructure has been implemented for harnessing challenges in the processing, management, analysis, and access of these valuable scientific assets. In our view, a first step towards the realization of such an infrastructure was the transition from a silos centric organization where different computing platforms rarely worked well together towards a more integrated, data oriented environment where various types of workloads are supported and data can be accessed from all computing engines efficiently. The deployment of the latest system, PICO, the improvement of the storage capacity and capabilities, and the reorganization of the network connectivity have represented an extremely important milestone in the implementation of a data centric vision. The new infrastructure supports seamless access, use, re-use of data, various classes of applications ranging from High Performance Computing to High Performance Data Analytics, data post-processing and visualization. Data produced on the FERMI system can be easily post-processed using PICO resources, stored in a long-term archive, shared with other scientists, and - if requested - re-analysed again to extract new insights. Our belief is that the new data oriented infrastructure would become a valuable asset for Italian and European scientists while supporting an open science policy. Optimizing the access to data is also a key factor to enable multi-disciplinary research thus reducing the duplication of effort and cost while accelerating scientific progress.

Daniela Galetti, Giuseppe Fiameni
Cineca

PICO: Big Data HPDA system

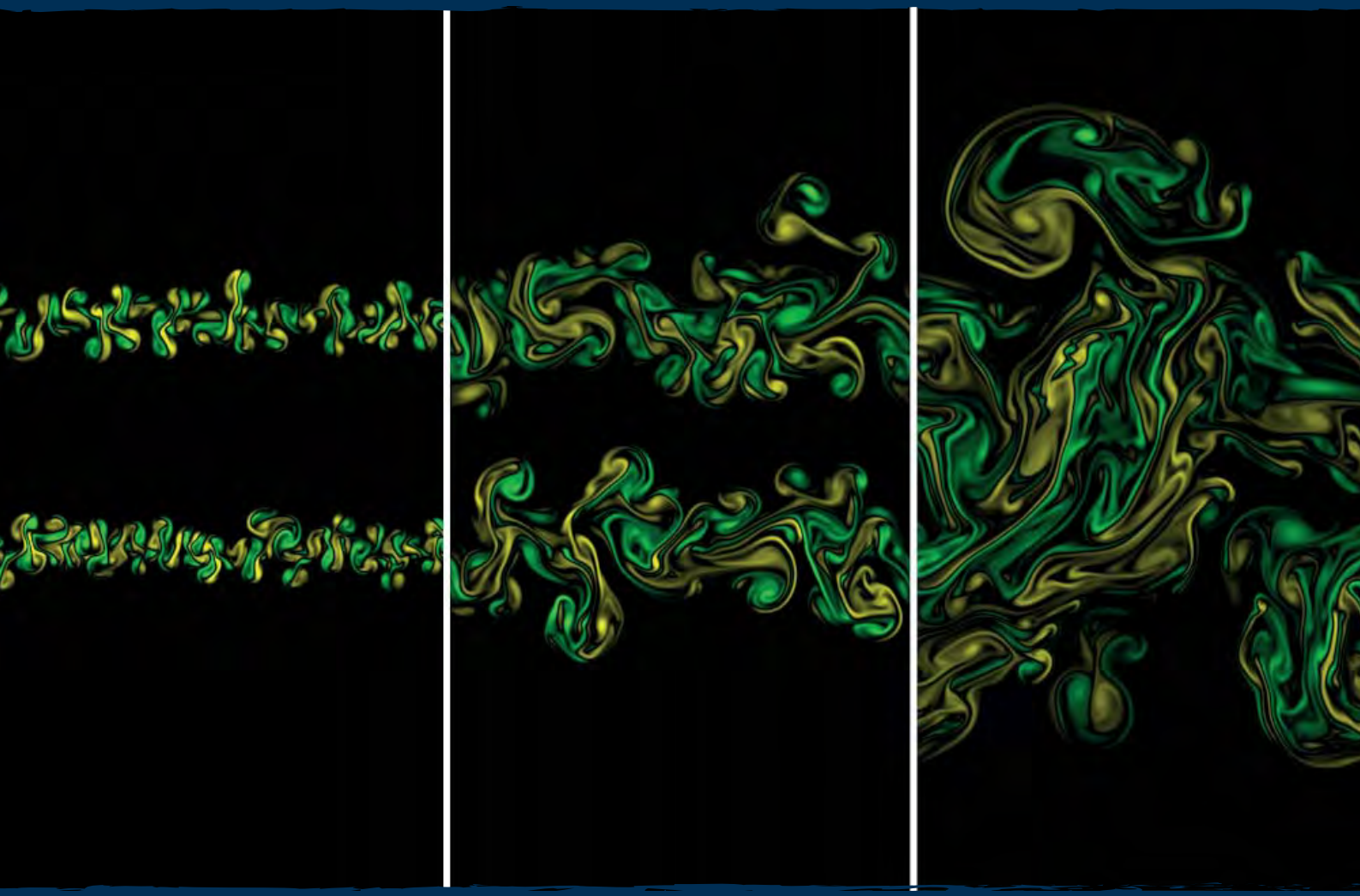
PICO is designed to embody the data-centric view of Cineca, moving from computers that compute (compute-centric), to computers that can extract information from large volumes of structured and unstructured data.
The new infrastructure aims at responding to the ever-growing demand of services and capacities (storage, management, compute, and visualization) which are essential to address the challenge of "big data" problems, nowadays a key factor of many scientific disciplines. The system is devoted to data intensive computing cases and complies with the peculiar hardware characteristics (large memory per node, massive storage equipment and sharing, fast data access and transfer, etc.), software tools (Hadoop, R) and the high-throughput techniques needed by data-oriented projects.
With the installation of Apache Hadoop, a framework for storage and large scale processing of data sets on clusters, Pico is able to provide the researchers with a powerful environment to help them manage and interpret large and complex datasets.
The processing power combined with access to sophisticated software packages enable researchers to harness the potential of supercomputing for the analysis of Big Data and can be used for anything from predictive analytics, social media analytics and text analytics to disease detection, prevention and treatment; financial modeling and smart energy metering.
Pico represents therefore also an opportunity for widening the user base to research domains that previously, in a pre-big data era, didn't have the need of enabling infrastructures such as economics and the social sciences. New expressions of interest actually come from the manufacturing industry, the Italian National Institute of Statistics (ISTAT), Bocconi University, etc.
A new range of services, not traditionally included in the HPC services, will be provided, specifically in the analytics domain, including the support on data mining and statistical software (Mahout, Knime, R, Stata, …) and the expertise on machine learning, data mining, predictive modeling, text mining, data pre-processing and data visualization for targeted applications development.
In this respect Pico is meant to drive innovation in the users' processes and in the way HPC infrastructures are used. This will be done through specific actions along some key directions such as starting new projects, setting new agreements and allowing new users to access and benefit from the infrastructure.
In particular the projects that will be hosted on Pico will address critical challenges for data management, data analytics, or scientific discovery impacted by the processing of vast amount of data, either structured or unstructured. A few of them have already been identified: EPIGEN (www.epigen.it),Human Brain Project (http://www.humanbrainproject.eu/). Another project, in a totally different domain, i.e. in the Finance field, will provide Stock Exchange data to researchers together with the computing facilities that enable the data intensive processing, including simulation and development of alternative scenarios. These projects will be treated as use cases for the concrete adoption of the new data-centric approach and will help defining the best way to structure future data services (e.g. as SaaS or IaaS).
In parallel, entities interested in participating to this new challenging transformation process will be identified (in the scientific field, in the industrial field, as well as in the public field) and new partnership will be reinforced to join efforts and take advantage of complementary skills and resources.

Roberta Turra
Cineca

INFN and Cineca: a fruitful collaboration

The years 2013 and 2014 have witnessed a large and fruitful collaboration between Cineca and Istituto Nazionale di Fisica Nucleare (INFN), the national research agency focusing on the study of the fundamental constituents of matter.
This collaborative work, that develops within the framework of a formal Memorandum of Understanding, is an obvious sinergic action: INFN has a large group of scientists working in areas of theoretical physics where access to large computing resources is of paramount importance while Cineca is the largest provider of HPC resources for the scientfic community in Italy.
Common work has developed in many different areas; in this note we only cover a few significant examples.
Researchers at INFN have used a large fraction of the compute cycles available on Fermi for several research projects at the forefront of theoretical computational physics. An area in which Fermi has been a key enabler of scientific results is Lattice-QCD, the computational approach to the study of the quantum field theories that describe the interaction among hadrons (a class of elementary particles). Almost equally important has been the collaboration in the area of computational fluid dynamics, where INFN researchers have a recognized leadership in the development and implementation of numerical algorithms in the framework of the Lattice Boltzmann method. These applications have a large amount of available parallelism that is almost fully exploited in our codes, so Fermi is an extremely efficient machine for these studies. We would also like to remind that INFN groups have been early users of the Fermi system; INFN codes have run on the machine just a few days after it was installed in summer 2012, giving an important contribution to the test and validation of the system.
Cineca and INFN have worked together in the framework of the INFN - SUMA project, that foresees a large spectrum of support activities for theoretical computational physics. In this context, several important common developments have looked at the most efficient strategies to adapt and improve numerical algorithms and code for new generation HPC systems, based on unconventional architectures, such as GPUs or many-core accelerators. This is a strategic area of development with hopefully important returns that will enable Cineca to take better strategic decisions on its future systems and INFN to use those new machines efficiently.
A clear proof of the level of mutual confidence among the two institutions is the common decision - made in spring 2014 - to combine resources for the procurement of a new common Tier-1 HPC system, that is currently being installed at Cineca. INFN provided a significant fraction of the funding for this project.
In this arrangment the new machine is operated by Cineca while INFN has partial access to these resources that add to INFN ability to produce fresh physics results.
Last but not least, Cineca and INFN are working towards the preparation of several applications for the Horizon 2020 EU programme. If these projects are approved, they will further contribute to the ties between INFN and Cineca and further propel our collaboration in an international context.

Raffaele Tripiccione
INFN and Ferrara University



This false-color picture shows the gradual development of vorticity (a measure of the degree of turbulence) in the time evolution of a Rayleigh-Taylor (RT) instability. The RT instability is triggered by a density difference in a fluid within a gravity field; the study of RT instabilities is important at the theoretical level and has several important applications in astrophysics, engineering and in the environmental sciences. The picture shows that larger and larger parts of the fluid domain behave in a turbulent fashion as the system evolves in time. This picture uses data from a science project done in collaboration between INFN and the Physics Department, Università di Roma “Tor Vergata” and using large computational resources provided by Cineca.

OGS: an historical cooperation on the Mediterranean ecosystem

The OGS numerical modelling groups hold an historical cooperation with Cineca in the use of HPC environments. OGS research activities, specifically in the fields of ocean biogeochemistry and seismological modelling, have extensively exploited the computational and storage facilities of Cineca, throughout the IBM series SP4/5/6 until the recent Blue Gene/Q, and the clusters BCX, PLX, EURORA. These activities have been developed in the framework of European and national projects such as MFSTEP, MERSEA IP, MyOcean, SESAME, OPEC, PERSEUS, MEDSEA, E-AIMS, INGV-DPC (V4, S3, S5, S1), CASHIMA (E2VP, E2VP-2).

In particular, within the MyOcean project a Service Level Agreement was signed between Cineca and OGS to professionally support the operations and management of the workflow that involves pre-processing, run production, post-processing, data archiving, and products dissemination to the MyOcean Information System for the short-term forecasts of the Mediterranean Sea biogeochemistry at 1/16° horizontal resolution. In addition, a recent activity has involved the implementation of the data repository of EMODNet Chemistry 2 on the cloud infrastructure made available at Cineca: the resources requirements were discussed and three environments are going to be set up, one for each visualisation service and one for the database. The system will enter in production on January/February 2015.

The need of high-level computational and storage resources for institutional and EC-granted research activities is however rapidly expanding due to the development of increasing data-intensive numerical codes used in the oceanographic physical-biogeochemical and seismological applications. The modelling activities are indeed oriented to increase the spatial resolution and the complexity of the representation of physical phenomena in the algorithms. This is essential, for example, to improve the simulations in coastal areas, with important economical and social added values. To accomplish such challenges, HPC resources and technological support are key requirements.

The targets of these applications mainly cover modelling of climate multi-decadal simulations and operational services for the living ocean, seismic risk assessment and mitigation, and analysis of experimental geophysical observations. Significant impacts of the large amount of data produced rise from the research and development activity for the marine biogeochemistry, spanning from the short-term forecasts to decadal reanalyses and climate scenarios, to the model uncertainty assessment through sensitivity studies. These are strategic in responding to the growing requests of reliable physical and biological marine data sets for the present and the future conditions rising at national and European level from political and social communities (e.g. the Marine Strategy Framework Directive). State-of-the-art activities include the ecological operational services, which aim at providing a model-based predictive platform for ecosystem management and fisheries.

Considering the seismological modelling, the major impacts concern seismic exploration, seismic hazard analysis, volcano seismology, seismic tomography and seismic source studies. In this field we recently started a study aimed at the development of HPC tools for the automatic recognition and localization of microseismic events, which is of increasing interest due to the growing perception of the risk related to the induced seismicity.

As important side activity, OGS and Cineca, aware of the rapid innovations which involve the growing heterogeneity of the HPC architectures, the increasing complexity of the scientific computing, and the consequent broadening of the gap between scientists and HPC professionals, have established, with the support of the Italian Minister for Education, University and Research, the program “HPC Training and Research in Earth Sciences (HPC-TRES)” to assist PhD/master students and PostDocs in improving their knowledge of the HPC tools for Earth Sciences applications.

Stefano Salon
OGS

OGS Explora in the Ross Sea (Antarctica) in the austral summer 2005-2006 during the 21st PNRA (National Antarctic Research Program) expedition.

INAF: Solving a Very Large-Scale Sparse Linear System with a Parallel Algorithm for the Gaia Mission

Gaia is an ESA (European Space Agency) mission whose main goal is to produce a 6D map of about one billion objects in our Galaxy and beyond, i.e. 3D positions (angular coordinates and parallaxes) and 3D velocities (proper motions and radial velocities). This map, for the first time, will extend over the whole Milky Way, and it will reach unprecedented accuracies at the 10-100 micro-arcsecond level (magnitude dependent) thus improving by a factor 100 on the accuracy and by 104 on the number of objects provided by Gaia's predecessor, the Hipparcos satellite. The satellite was launched on 19 December 2013, and it has just started its 5-year operational period after completing the initial in-orbit calibration, or (as it is usually refereed to) commissioning phase.

While ESA took charge of both launch and satellite construction (including the payload) the national agencies are providing the needed effort for the equally challenging task of data analysis and reduction. The Data Processing and Analysis Consortium (DPAC) is a consortium of about 500 scientists (mainly European) organized in 9 Coordination Units and 6 Data Centres.

The Italian contribution, thanks to the support of both ASI (the Italian Space Agency) and INAF (the National Institute for Astrophysics), is twofold: Italian scientists are involved in the data processing of non-Italy-based data centres, while at the same time Italy hosts a Data Centre (the DPCT) dedicated to running the software provided by the Italian Development Unit called Astrometric Verification Unit (AVU) and of some other dedicated experiments. In particular, the AVU is in charge of providing a solution of the Global (Astrometric) Sphere Reconstruction (GSR) alternative to the baseline analogue, named AGIS (Astrometric Global Iterative Solution), and to check the compatibility of the two solutions. This is a fundamental step for the scientific qualification of the Gaia astrometric results.

Originally GSR was foreseen to solve a sphere of one to some (possibly ten) millions of stars, but thanks to a research agreement between INAF and Cineca, the latter became part of the Italian DPCT by providing access to its HPC resources for the Gaia project. In particular the most computationally-intensive part of GSR, namely the module that solves the system of linear equations necessary to compute the new coordinates, will run on the IBM Blue Gene/Q "Fermi". This gave the Italian contribution a "quantum leap" which brought the GSR solution at the same level of that of AGIS, i.e. to a sphere of 50 to 100 millions of stars.

Such an effort, which implies the solution of a system of about 10^{11} rows (observations) by $5 \bullet 10^{8}$ columns (unknowns), required the implementation of specialized parallel code using a mixed MPI+OpenMP paradigm implementation of the LSQR algorithm. Development of this formidable code was a joint effort of INAF specialists from both Catania Astronomical Observatory and Torino Astrophysical Observatory, with continuous support provided by the Cineca experts.

Current tests suggest that a sphere of 100 million stars can be solved in 10 to 20 days by running the sphere reconstruction module on 2048 nodes of the Fermi supercomputer.

We cannot wait to run the first large GSR on Fermi early next year, when a sufficient number of Gaia data covering the entire celestial sphere will finally become available!

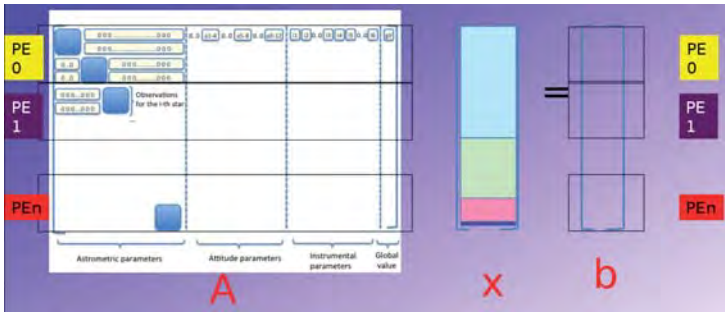


Figure 1: memory distribution among the Pes (nodes of the IBM BG/Q) of the coefficient matrix (A), known terms (b) and unknowns (x) in the parallel code.

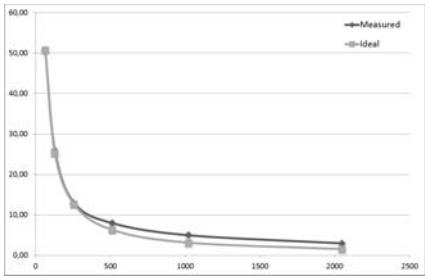
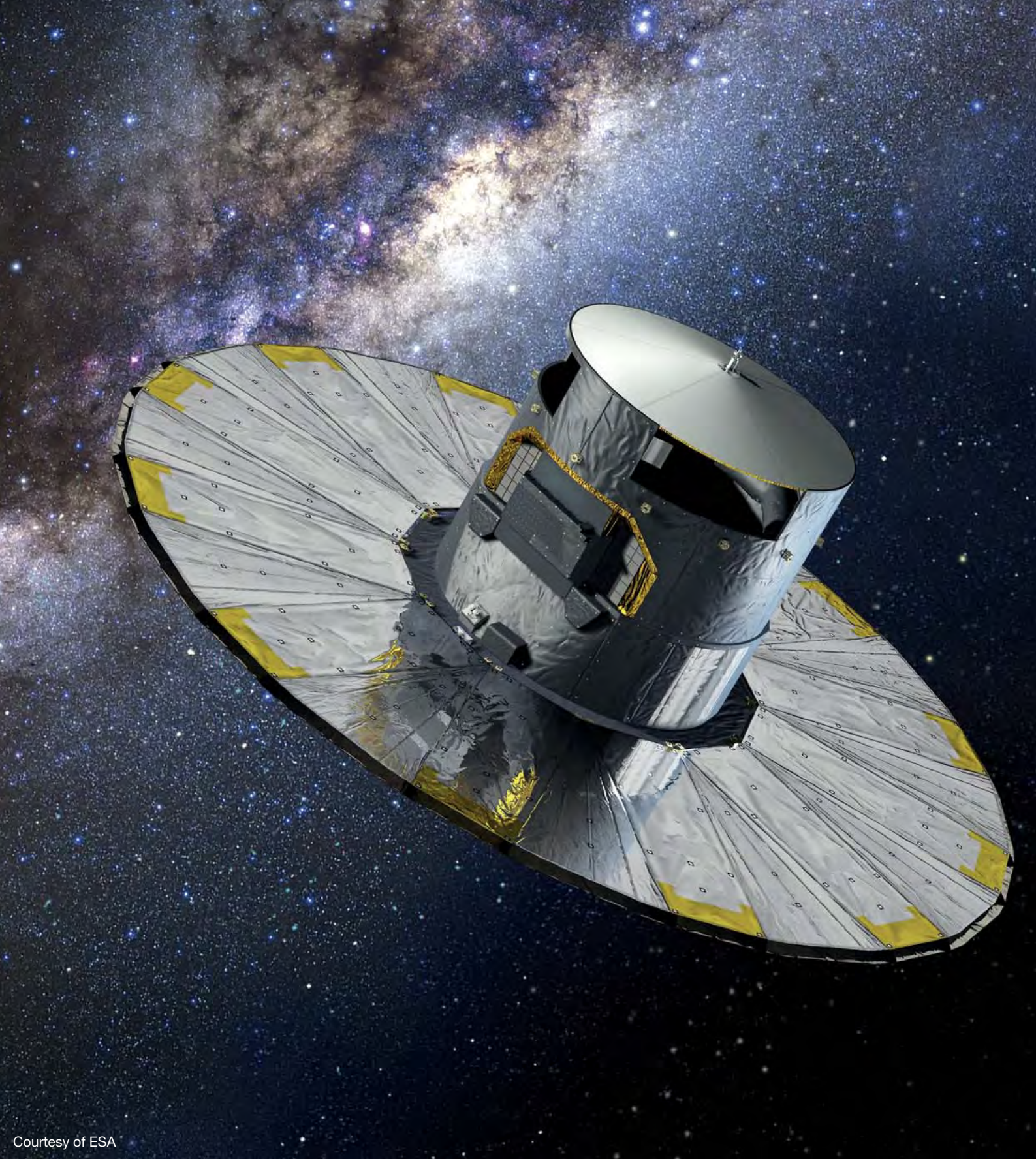


Figure 2: code scalability up to 2048 nodes. The curves show seconds-per-iteration (vertical axis) vs number of computing nodes.

Ugo Becciani, Alberto Vecchiato, Mario G. Lattanzi
INAF



Courtesy of ESA

ICTP: HPC advanced training for developing countries scientists

For more than 50 years, the Abdus Salam International Centre for Theoretical Physics (ICTP) has been a driving force behind global efforts to advance scientific expertise in the developing world. A UNESCO Category I institute, the ICTP is a centre for advanced training and research in physics and mathematics that has helped scientists from developing countries overcome their isolation and contribute to state-of-the-art research.

Each year, ICTP hosts more than 6,000 scientists from developed and developing countries. Each year, ICTP organizes more than 60 international conferences, workshops, and numerous seminars and colloquia on subjects ranging from elementary particle physics to cosmology, condensed matter physics to material science, mathematics to computational physics, geophysics to climatology, biophysics to medical physics, laser physics to nonconventional energy sources, scientific computing to collaborative development for large-scaling scientific packages, including parallel programming and training on HPC.

ICTP's strategic plan looks with particular attention at scientific computing as an indispensable tool in research. ICTP fosters educational programs and activities aimed to consolidate the technological background needed to master state-of-the-art hardware and software for scientific applications. Co-organized with SISSA, an innovative Master program in High-Performance Computing (MHPC) is today listed among the ICTP programs. In the last two years Cineca's support of this activity has been extremely important. With the help of Carlo Cavazzoni, Giuseppe Fiameni and Giorgio Amati, Cineca has actively collaborated in co-organizing and lecturing within international workshops, advanced schools for scientific programming, symposiums on data-intensive applications and the new MHPC. The participation of Cineca's qualified staff members adds value to all activities thanks to their experience, their vision on high-end computing and their detailed knowledge of advanced parallel programming techniques for large-scale scientific applications.

Moreover, for the ICTP scientific community, Cineca represents an opportunity to access a world-class supercomputing facility for their research activities. ICTP scientists in the Condensed Matter and Astroparticle Physics groups regularly exploit Cineca HPC resources to study problems in their fields of research. In this regard, it is also extremely relevant for ICTP's scientific community that Cineca participate and contribute to PRACE (Partnership for Advanced Computing in Europe).

Ulrich Singe
ICTP

CNR and Cineca-SCAI: a success story

CNR has been enjoying a fruitful and successful collaboration with Cineca-SCAI department, particularly in the field of materials applications, for many years. This has given our researchers the possibility to keep the pace with the evolution of HPC high-end systems, in terms of software tools and in terms of scientific productivity, thus determining major competitive advantages.

I will just give a couple of examples. Among the successful collaborations in software development, we developed a joint effort (Cineca-SCAI with two CNR institutes: CNR-Ism and CNR-Nano) to implement a new parallelization strategy in the Yambo (http://www.yambo-code.org/) code: this led to an enormous improvement of the performance of the code, permitting to scale up to more than ten thousands cores. With this achievement this code, developed at CNR, is getting ready for the next generation HPC hardware and suitable for fully ab-initio calculations of electronic and optical properties in realistic systems.

A further example of fruitful collaboration on applications and research is certainly the joint work on ab-initio nanotribology (Cineca-SCAI with CNR-Nano, http://www.nano.cnr.it/) which led to greatly improved codes. Thanks to this effort, the group of MC. Righi was among the first in developing ab-initio molecular dynamics for realistic tribochemical reactions: this is allowing CNR to develop relevant industrial collaborations e.g. in the automotive and lubricants sectors.

Cineca-SCAI and CNR have worked together along the years to build knowledge transfer initiatives toward motivated young researchers, who have become themselves HPC application experts with an high level of success in peer-reviewed grants for accessing high-end international resources like PRACE in Europe and Oak Ridge National Laboratory in the USA. Through close interactions with SCAI, our graduate students and post-docs acquired HPC competences which greatly contributed to make their curricula more appealing. Collaborations on advanced schools in computational materials science organized by CNR researchers were very valuable and much appreciated.

We are looking forward to growing collaborations in the next years, especially towards the exascale evolution of our codes. A joint effort is also being started in the direction of a European initiative on HPC applications for materials. Both directions are pursued also through joint participation of Cineca and CNR institutes in EU proposals, which are certainly reinforcing the leading international role of our community and will hopefully provide substantial support to Cineca, CNR, and the broader Italian scientific community in the future.

Elisa Molinari
CNR Istituto Nanoscienze, Modena
Modena and Reggio Emilia University

CNR-INSEAN: CFD reconstruction of the Jolly Nero accident

On May 7th, 2013, during her manoeuver to leave the port of Genua – assisted by two tugs, the "Spagna" and the "Genua" – the tanker ship "Jolly Nero" hit the control tower of the harbor ("Nuova Torre Piloti") leading to its collapse (see figure 1 and 2). The accident caused nine casualties and four wounded. As the Prosecutor required to CNR-INSEAN to reconstruct the dynamic of the accident, HPC activity was necessary to analyze trajectories, forces and moments acting on the many vehicles involved in the tragedy. The main HPC activities carried out are described in the following, whereas results and findings will not be presented nor discussed being still classified.

For the reconstruction we started from collecting all the available inputs, including (i) audio recording from the Simplified Voyage Data Recorder (SVDR) on board of the "Jolly Nero"; (ii) geometrical description of the "Jolly Nero" including her appendages (propeller, rudder, anti-roll fins, bow thrusters), her sinkage and trim values at the departure, and power characteristics of the propeller and of the thrusters; (iii) time history of the position of the "Jolly Nero", as obtained from the GPS and the compass; (iv) time history of the rudder movements, as well as of the orders for the propeller, the bow thrusters and to the tugs; (vi) geometry and maximum power of the "Genua" and "Spagna" tugs. Position and kinematic parameters of the tugs were known only for some time periods during the manoeuvers, from video recording and from the Automatic Identification System. Planimetry and bathymetry of the Genova harbor were also available from the Port Authority.

For the estimation of the forces on the ship, bollard forces (strength and direction) and position of the tugs, the computation of the hydrodynamic loads on the "Jolly Nero" during the maneuvering is mandatory. Hydrodynamic loads have been estimated by numerical simulation of the ship undergoing the prescribed manoeuver (as recorder by the GPS and the compass) in the Genua harbor.

Simulations have been carried out by means of a suitable CFD solver based on the discretization of the unsteady Reynolds averaged Navier-Stokes equations. The solver employed is the Xnavis code, a general purpose CFD solver entirely developed at CNR-INSEAN. Xnavis is a Fortran 90 code featuring an efficient parallelization based on MPI and OpenMP paradigms. The hybrid parallelization is crucial to efficiently run on machines with several cores, such as the IBM Blue Gene/Q FERMI at Cineca, which has been used to run the numerical simulations. The code is highly efficient and optimized for this kind of architecture; indeed, prior to the application described here, the code has been profoundly revised in order to properly scale on massively parallel systems, such as PRACE Tier-0 systems. Researchers of the CFD department of CNR-INSEAN applied to a PRACE Preparatory Access C to have direct support from PRACE experts to optimize and overcome technological challenges related to scalability on thousands of processors. The Preparatory project was successfully finalized on October 2013 and, thanks to the work performed in that context, including the support by Cineca experts, the obtained scalability was rather satisfactory.

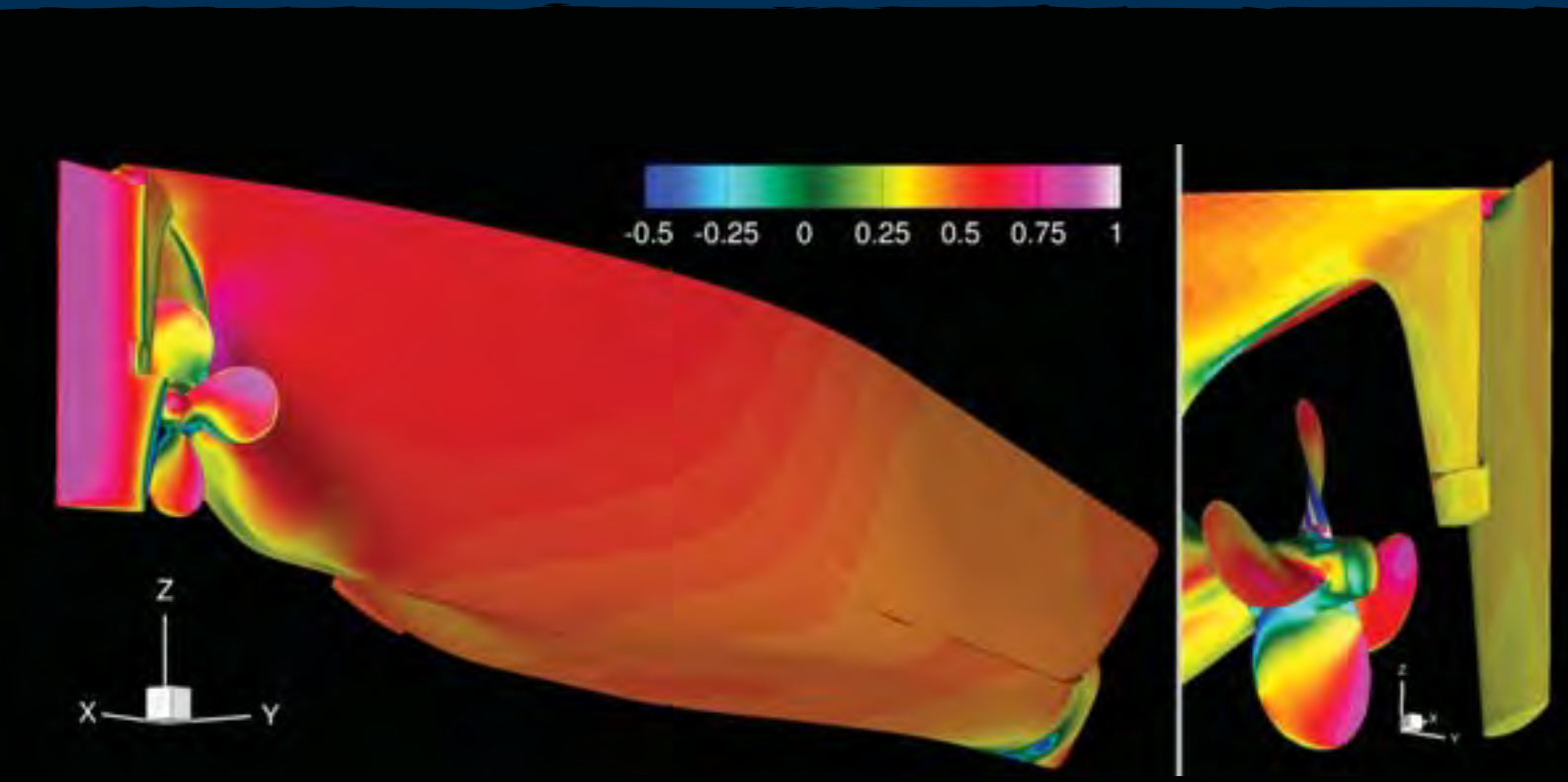
Simulations were carried out taking into account all the geometrical details of the ship, including the rudder and its movement, the bilge keels and the propeller (see figure 3). Moreover, in order to taken into account for possible shallow water and confined water effects, the manoeuver of the tanker is simulated in the harbor; water depth variations, in particular close to the quayside below the control tower has been also considered. Due to the level of details that has been considered (the physical domain is discretized by about 20M of grid points), the need to simulate the complete manoeuver (starting from the acceleration phase in the channel and the turning in the maneuvering basin, up to the instant of the impact) and the limited resource time available connected to the schedule of the process, computations have been highly demanding. Computations have been ran on the IBM Blue Gene/Q FERMI machine made available by Cineca. Typical computation required about 96 wall time hours on 4096 cores for the computation of about 15 minutes in real time. Several computations have been performed in order to both assess the uncertainty of the numerical simulation (such as the grid dependency and the effect of the regularization of the input parameter) and to investigate different operational condition, the possible effect of very shallow water due to the presence of sediments, the effect of the rudder actuation and the actuation of the bow thruster). The reconstruction of the manoeuver has been completed; results are consistent with the observation, and the role of the uncertainties associated with the input parameters (e.g. GPS position is affected by some uncertainty). Simulations have been completed within the time allowed and have been delivered to the public prosecutor; results are under investigation and discussion.

Riccardo Broglia, Stefano Zaghi, Roberto Muscari, Giulio Dubbioso
CNR-INSEAN

Figure 1: Aereal view of the pilot tower remains.

Figure 2: Reconstruction of the leaving port manoeuver.

Figure 3: Overview and stern details of the surface pressure on the hull and appendages.



INGV: Numerical simulation of explosive volcanic eruptions

Explosive volcanic eruptions are among the most dangerous natural phenomena. In Italy, about 2 millions people are at risk from explosive volcanoes, particularly from Vesuvio, Campi Flegrei and Ischia potential reawakenings. Complementary to the study of past behaviour of volcanoes (subject of geological studies) and to continuous monitoring of subsurface and surface manifestations of magmatic activity (e.g. geophysics, geochemistry, etc.), numerical modeling of explosive scenarios is becoming a fundamental pillar of volcanological research as well as of volcanic hazard assessment and risk mitigation. In this context, the main objective of forward numerical modeling of eruption dynamics is the prediction of the impact of plausible future eruptive scenarios through the integration of the available geological and geophysical information into reliable physical models.

In the last years, the improvement of numerical discretization techniques, solution algorithms and high-performance computing codes, linked to the augmented availability of supercomputers, have made the simulation of complex, large-scale volcanic scenarios even more feasible and attractive. However, the most challenging issue for the simulation of realistic eruptive scenario is still probably related to numerical resolution associated with multiscale processes. Explosive eruptions develop indeed over a broad range of spatial (and temporal) scales and their large-scale dynamics (developing over tens of kilometers or more) are extremely sensitive to processes occuring at the scales of the vent (i.e. tens or hundreds of metres), down to the particle size (below one millimetre). On the other hand, very different regimes characterize the dispersal of eruptive products, ranging from supersonic flows near the vent, to turbulent atmospheric transport far away from the source, to the viscoplastic flow of dense granular avalanches travelling along the volcano slopes. Finally, the fractal nature of three-dimensional natural topography makes the simulation of surface flows extremely sensitive to numerical accuracy and resolution.

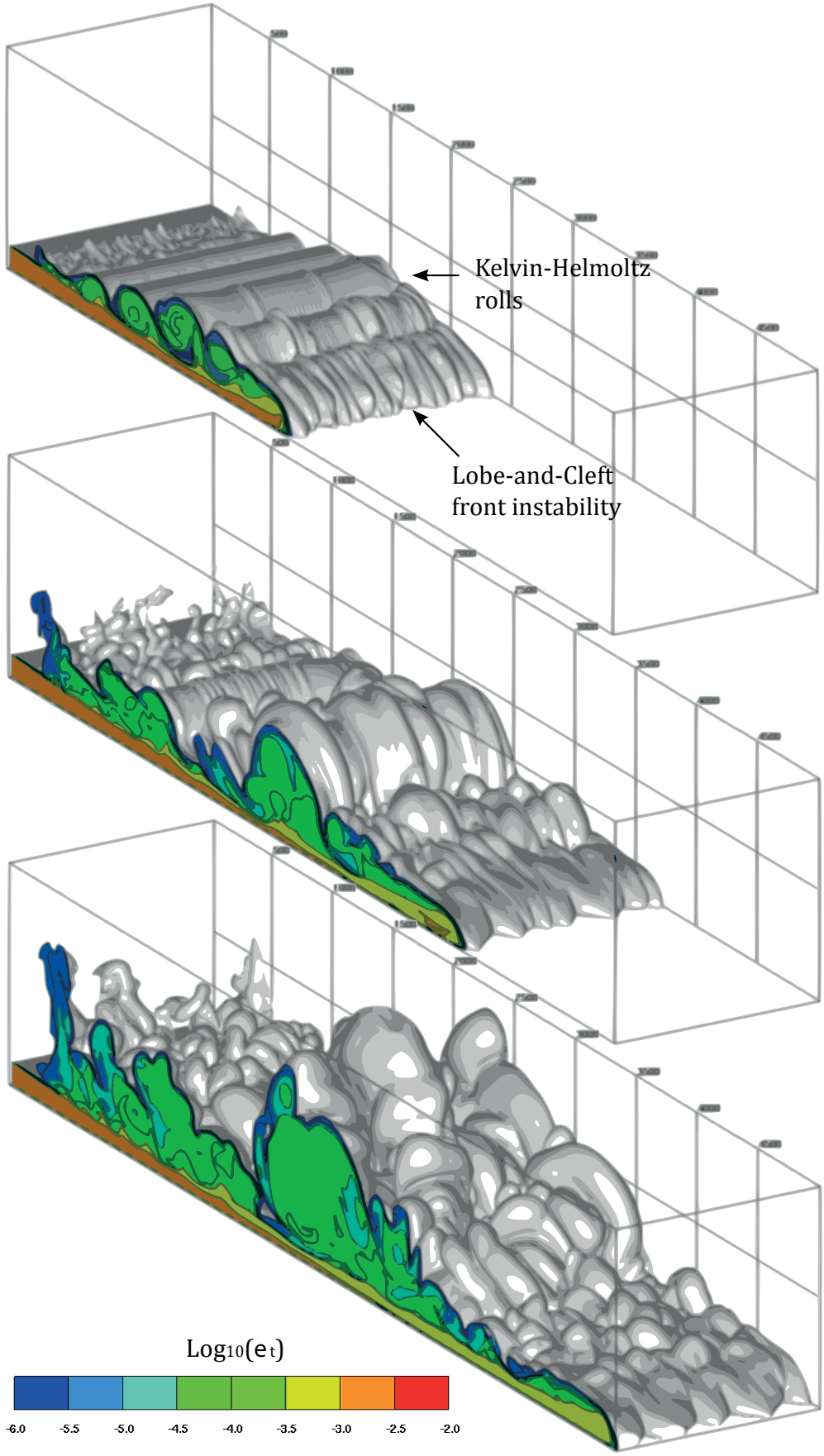
Simulation efforts have so far mostly focused on describing the dynamics of subsystems (for example, volcanic plumes, Fig. 1 - and pyroclastic flows, Fig. 2), only accounting for the one-way coupling between different spatial domains (e.g. magma chamber, volcanic conduit and edifice, eruption plume, surface pyroclastic flows, atmosphere).

Three-dimensional numerical simulations have allowed to unravel some key aspects of the physics of gas-particle turbulence in buoyant volcanic plumes and to quantify the effect of particle sedimentation and current stratification on the mobility and runout of hazardous pyroclastic density currents. In these applications, modeling of subgrid-scale dynamics represents the main physical and numerical challenge, since the governing non-linear systems of partial differential equations may exhibit complex interplay among wavelengths.

In this framework, predicting the potential impact of a target plausible eruptive scenario on the anthropic and/or natural environment (Fig. 3, La Soufrière of Guadeloupe) is particularly challenging and critical, especially in those cases where numerical outcomes are used to support decision making. This is even more true when considering the fact that a rigorous model validation in volcanology (and more generally for many other geological systems) is highly problematic, due to non-repeatability of observations, unsteadiness of the system, incomplete knowledge of data and consequent possible non-uniqueness of model solutions. Also in this case, however, supercomputing can greatly help picking our way through, by allowing wide sensitivity analysis and statistical sampling of a credible range of input parameters, thus driving a main future “change of paradigm” towards a computational volcanic hazard assessment.

INGV also coordinates the EPOS initiative (http://www.epos-eu.org/), one of the most important European research infrastructure in the field of the solid Earth Sciences. In the course of the 2015, EPOS will be legally established in Italy using the ERIC framework and enter its implementation phase for the design and implementation of infrastructure services. To this respect, EPOS will collaborate, among other European large scale facilities, with Cineca for the provisioning of technical support and resources both as national contribution and as part of larger European infrastructures such EUDAT and PRACE.

Tomaso Esposti Ongaro, Matteo Cerminara, Augusto Neri
Istituto Nazionale di Geofisica e Vulcanologia



Three-dimensional numerical simulation of a turbulent pyroclastic density current fed by a steady-state inlet flow. The isosurface of gas temperature at T=100°C highlights the progressive development of the Lobe-and-Cleft (LC) and Kelvin-Helmoltz (KH) instabilities of the flow front and upper interface, which drive turbulent mixing and air entrainment. Progressive current unload occurs under the effect of gravitational settling of particles, leading to buoyancy reversal and rise of convective clouds. Simulations performed with the non-equilibrium multiphase flow model PDAC (Esposti Ongaro et al., 2007).

Cineca and the University of Bologna: together for developing High Performance Computing

2014 marked an important moment in the collaboration between the University of Bologna and Cineca, namely the signature of a 5-year framework agreement for the development of High Performance Computing.

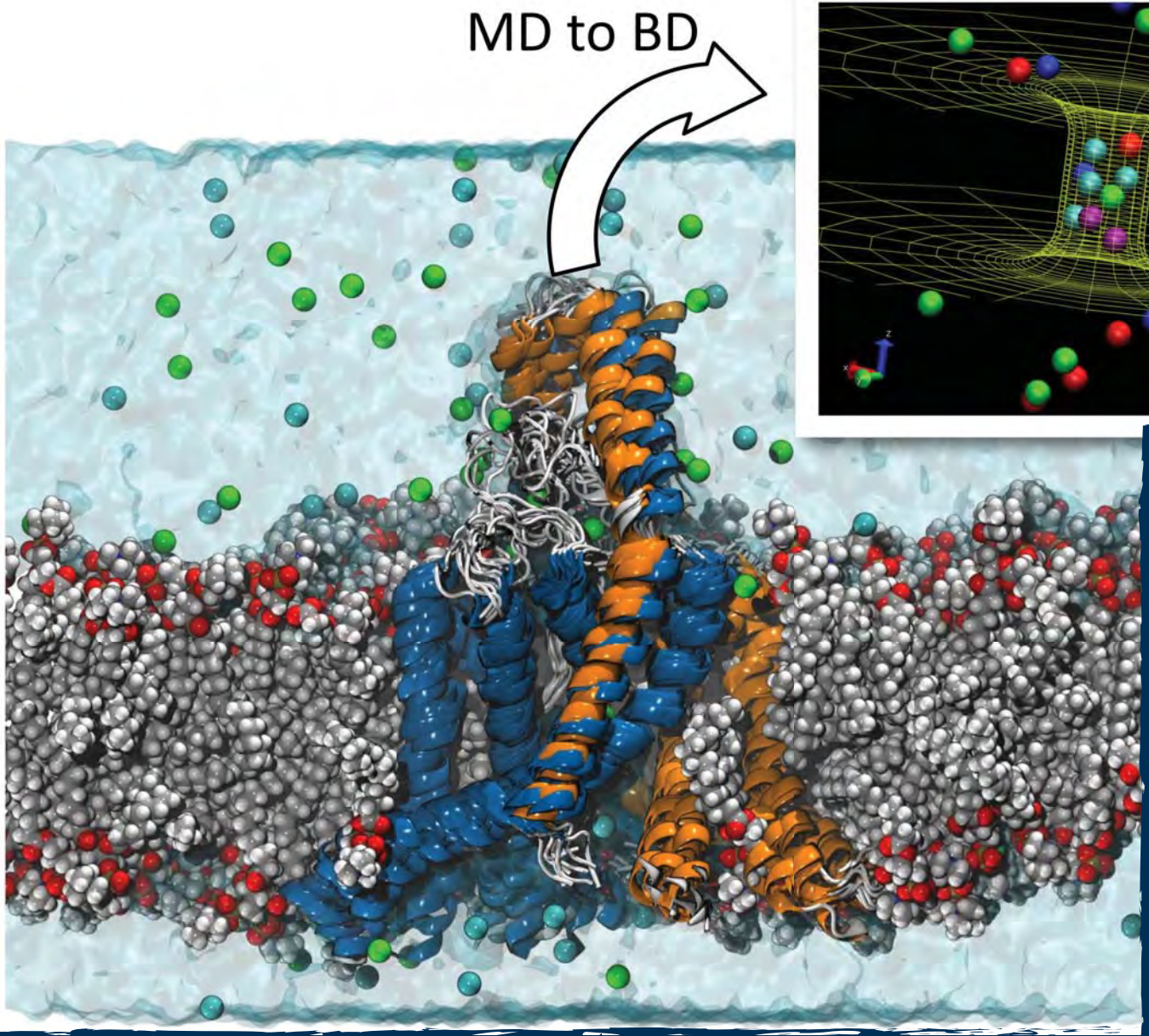
Already in the last years, the University of Bologna and Cineca had launched a number of specific scientific collaborations in the framework of HPC. It is not therefore by chance that the two institutions have decided to consolidate their relationships through a more structured partnership, able to benefit also of their geographical proximity in order to fully seize all opportunities related to joint research activities, as well as the possibility to develop joint projects and initiatives at the local, national and European level. The final goal is that of combining scientific research with the development of higher education paths, technology transfer, the promotion of new services and new entrepreneurship, the attraction of resources and investments, also at European level, the dissemination of research results.

The ongoing collaborations in the context of HPC include the development of advanced computing systems with high energy efficiency, the multiscale simulation of pharmacologically relevant ion channels, the infrastructures supporting calculation systems for big data processing, Cloud, stream processing, and smart cities.

The interests of the University of Bologna with regard to High Performance Computing are huge. With its wide interdisciplinary characterisation, the University can count on excellent competences and is carrying out research activities that can, on one hand, contribute to the technological development of the HPC infrastructure (hardware and software), on the other, it can benefit of supercomputing in several and highly diversified application fields: physics, biology, pharmacology, astronomy and cosmology, material engineering, nano and bio-technologies. Furthermore, the University of Bologna is member of the ETP4HPC - European Technology Platform for High Performance Computing. The collaboration with Cineca, one of the most important actors at European and world level, present in the ranking of the world most powerful supercomputers, is therefore strategic for the University.

Supercomputing is more and more considered at international level as a key enabler for the progress of knowledge; it is particularly important for the development of scientific research as it can be used for simulating complex systems such as those connected to weather forecasting or to the cells, and it can be employed for processing huge amounts of data in several applicative fields, from smart cities to personalised medicine, simulating real life behaviours. HPC also plays an essential role in the European research and innovation policy, where it is part of the priorities set by the Digital Agenda for Europe.

Verdiana Bandini
Bologna University



Schematic representation of the multiscale approach to compute the conductance of ion channels on varying conditions of transmembrane potential and salt concentration. The atomistic simulation is employed to gather information on the dynamic behavior of the TRAAK potassium channel (K_{2P} 4.1). The ensemble averages calculated at this level of description are then employed by the Brownian Dynamics simulator to explicitly simulate ion transport.

Smart city scenario where Big Data and a moltitude of data streams are produced and collected through sensors and mobile devices; high performance computing is required for real-time data processing, in order to collect, assess and actuate rapidly appropriate control actions.

ALMA MATER STUDIORUM
UNIVERSITÀ DI BOLOGNA

UNIBO: towards high energy efficient HPC systems

We are collaborating with Cineca since 2013 with an ambitious research project on improving the energy-efficiency of future supercomputing by applying run-time management techniques and methodologies typical of Embedded System. This was in our research agenda since 2009 when we started a research collaboration with Intel Lab Braunschweig and scaled-up 2012 with the Multitherman ERC advance EU project. Since 2013 Cineca opened its facility doors to our group and we started a set of technical actions.

Instrumenting the Eurora supercomputer with a fine-grain HW/SW monitoring infrastructure to create a single collecting point for facility and machine measurement as well as Job dispatching and progress tracking. This infrastructure has been integrated with a tool for the direct measurement and reporting of the Energy-to-Solution of job executed on the supercomputer. This technology has been an enabler for a deeply understanding the real SW/HW evolution and interaction of first-class supercomputers. This activity has directly produced as outcome a Technology Transfer Award from the Hipeac community in 2013 and a paper accepted at DATE conference presented in Dresden in march 2014.

We have conducted a massive measurement action for characterizing and generating ground-knowledge on the energy/performance optimization spots in the Eurora Supercomputer. This has brought to a paper presented in ISLPED conference in San Diego in August 2014 and a best poster Award in 2014 at the Workshop of Energy Efficient Electronics and Applications held in Lausanne in January 2014.

We have started the study on how to improve the performance of commercial job dispatcher by introducing performance, thermal and energy models in the problem formulation and solving it by using advance optimization strategies such as Constraint Programming. This activity have already led to a publication in the CP 2014 conference held in September in Lyon.

We have started the modelling and study of the cooling infrastructure and its optimization. This work have already conducted to an accepted paper at the DATE 2015 conference in the Green Computing track.

We have started the development of advanced SW thermal management techniques for controlling the thermal evolution of supercomputing machine while minimizing the performance impact of such evolution.

Overall the collaboration have fast scaled up in two years by involving three research groups spanning from the embedded system, to artificial intelligence and control theory with a direct contribution of one full professor, two associate professors, four post-doc, two research assistance and three PhD students and several master student. In the addition to the scientific outcome, the collaboration with Cineca and the day-by-day time spend by the UNIBO researcher inside Cineca has conducted to the growth of experience in the supercomputer domain and the presence in several HPC organizations as well as in several European founding action for the HPC development. As the matter of fact the collaboration with Cineca has opened new research challenges and already produced outstanding scientific outcome recognized by several international communities as well as novel didactic opportunities directly exploited in the study curriculum of information technology engineering student of the Alma Mater.

Luca Benini, Andrea Bartolini
Bologna University

CINI: software engineering and development of HPC applications

CINI and Cineca started in 2014 a scientific cooperation to better leverage on competencies available in the scientific community of Italian Universities, with special reference to advanced training in HPC.
CINI is the Consorzio Interuniversitario Nazionale per l'Informatica, a consortium of 39 public universities including almost all Italian research departments active in Computer Science and Engineering.
Cineca has a long tradition of organizing Schools in Parallel Computing and scientific software running on HPC architectures.
A small joint steering committee identified Software Engineering as a primary target of the cooperation. Indeed, Cineca, on the basis of its estabilished training tradition, perceived the need to embed a basic training framework in Software Engineering for HPC for Science and Engineering research in its training offer for young researchers using the novel HPC architectures.
A first event in which some software engineering topics were exposed to HPC research users was the Advanced School in Parallel Computing held in Bologna at Cineca headquarters in February 2014. In that event (a five-day course) a whole day was devoted to software engineering topics, presented by professors from the University of Bologna and the University of Milan-Bicocca. The topics were: a basic introduction to the software development process for scientific applications; and testing of scientific software for HPC. In this case the "students" were researchers expert in HPC software, who where especially interested by the topic of software testing.
After this initial event, a joint committee defined a basic syllabus to be taught over two days in the School of Parallel Computing, to be held in three 10-day editions each in Rome, Milan and Bologna. The syllabus was as follows:

- Introduction to software engineering: basic notions and terminology;
- The software development process in the case of HPC applications;
- Issues in publishing and maintaining research software and data;
- Basic architectural patterns for HPC software systems;
- Testing and analysis of research software;
- The quality of research software.

Attendance to this school was mainly from young researchers, master phd or post-doc students, with initial experience in software development for HPC architectures. They generally lack formal programming training, and have no experience in participating to multiperson development teams building complex software artifacts. Thus the definition of the syllabus was especially challenging.
The results of the first year can be summarized as follows: HPC users as software developers immediately understand the value of training in testing and quality. It is more difficult to attract them to some complex software engineering issues, like the variety of software development process models (Waterfall, iterative, agile) or modeling technologies like UML. They are instead quite reactive to design patterns for parallel programming or tools for version control and configuration management, useful for they daily research work.
On the basis of the feedback from the attendees to the training events, CINI and Cineca agree that the cooperation is a strategic asset for the Italian HPC community, and plan to better tune it in the years to come.

Marco Ferretti
Pavia University


CINECA
Data Management
Exascale
HPC Infrastructure
Resources Allocation
Community Code Activities
Solutions for Innovation
Meteo Climatology
Connectomics
EUDAT
RDA
RESEARCH DATA ALLIANCE
MONT BLANC
DEEP
PRACE
HBP
Astrophysics and Other Plasma Physics
Particle Physics
Life Science
CFD and Engineering
HPC distribution
Condensed Matter Physics
Computational Chemistry
Intel® PCC
SPECFEM 3D
UnipolSai
ASSICURAZIONI
FORTISSIMO
ETP 4 HPC
eni
Dompé
myOcean
PROTEZIONE CIVILE NAZIONALE

SECTION 3

2014 HPC IN NUMBERS: ASSESSMENT AND IMPACT

Our competences and skills

This section of the report has the aim to present the specific characters of the staff, which constantly supports and collaborates with our ecosystem, the scientific communities, the international projects, and the innovation partners.

The competences and professional skills on board of the perimeter of the SCAI Department is the result of a very synergic and complex continuous improving process, which combines education background, accumulated experiences and progressive training.

This variegate spectrum of knowhow is our offers to the national and European research communities to attack scientific and socio economical challenges at the forefront of the excellence.

First of all the educational background: considering the resources working on scientific computing activities, all the members of SCAI hold a university degree, many have a PhD graduate (23), and some more others have also a post laurea master. This high quality level of the educational background is constantly improved by mean of the participation to numerous R&D projects and scientific collaborations, besides a continuous attendance to training events and workshops, and HPC domain exhibits and scientific conferences. The vertical competences range from economical and law to mathematical, statistical and engineering, from physics and chemistry to informatics and biology.

Strong return of these investments is represented by a specialistic support, which addresses a multi domain interdisciplinary and multi disciplinary approach to address scientific investigations.

During 2014 SCAI department staff participated to 27 events presenting the results of their activities, 32 members of the department had a specific engagement and responsibility in leading R&D project tasks and coordinating collaboration actions.

Particularly important are the competences and the Project Management Professional Certification detained by the Project Management Office staff for the conduction of effective Research & Development and Innovation projects and to assure to reach the foreseen outcomes and deliverable objectives of the different activities. 6 persons detain the PMI certification.

The participation in the major R&D and infrastructural initiatives in Europe on one hand has meant an enrichement of our cultural baggage and has allowed us to make better choices with regard to new technologies (paths of technological development and selection as the one that brought to EURORA, or to the installation of Pico).

Important collaborations, such as the one with Intel as Intel Parallel Computing Center, as the presence in PRACE, allowed us to optimize application codes that have found an improvement in their performance and have been made available to the scientific community in their most powerful versions (QE, SPECFMD, GROMACS, etc).

As another exemple, the experience in the Epigen project allowed us to create a computing platform, ODESSA, made available in terms of service to the bioinformatics community and in perspective could become a service for a personalized medicine approach.

Experience in projects towards the exascale, as Deep and Deeper, Montblanc and Montblanc2 allowed us to deepen our skills in the integration of systems with accelerators and embedded components, important aspects for the evaluation of knowledge in the upcoming technological choices.

The presence of Cineca as one of six PRACE Advanced Training Centers put us in the position of being part of a synergisc action of high-level training standardized and validated at the European level and, on the other hand, to keep our knowledge updated day-by-day.

Along the time the skills and the knowhow on which the SCAI Department can count on contributed twofold in the overall trustworthiness of Cineca: on one side the capability of the SCAI Department staff to cope with intrinsic flexibility of the research processes, which by definition move forward upfront to the new discoveries, on the other side to guarantee the rigorous management of the peer review process for granting of computing resources.

The specific intangible of the human capital will be, during the next 2015, objective of a specific assessment action in order to keep pace of the training and experience acquisition needs, to maintain at the top level the quality of the available professional skills to effectively support the researchers activity.

Sanzio Bassini
Cineca

Talks

Carlo Cavazzoni: Trends and Perspectives for HPC infrastructures Lattice QCD and hadron physics
ECT, 14-17 January 2014 (Trento, Italy)

Carlo Cavazzoni: Eurora experience at 5th European workshop on HPC centre infrastructures
1-3 April 2014 (Bouray-sur-Juine, France)

Carlo Cavazzoni: Eurora experience at Workshop on Exascale and PRACE Prototypes: Lessons learned from Mont-Blanc, DEEP and PRACE
19 -20 May 2014 (Barcelona, Spain)

Carlo Cavazzoni: Performance and Energy Efficiency in Material Science Simulation on Heterogeneous Architectures
HPCS 2014, 21-25 July, 2014 (Bologna, Italy)

Giuseppe Fiameni: Exascale: challenges and opportunities in a power constrained world
Perspectives of GPU Computing in Physics and Astrophysics
Dept. of Physics, Sapienza Roma University, September 15-17 2014

Carlo Cavazzoni: Material Science and High Performance Computing, Challenges and opportunities
LET'S 2014, 29 September-1 October 2014 (Bologna, Italy)

Carlo Cavazzoni: MPI Communicators for model coupling and intro to the hands-on session
Lab-Session: Use of MPI Communicators for Modules Coupling (InfoLab)
ICTP, 27 October-14 November (Trieste, Italy)

Giuseppe Fiameni: EUDAT strategies for handling dynamic data in the solid Earth Sciences
27 April-02 May 2014 (Vienna)

Giuseppe Fiameni: Horizon 2020 : la disseminazione e la condivisione dei risultati della ricerca prodotta in Europa
I dati della ricerca nel contesto di H2020 e il contributo CINECA: verso una infrastruttura collaborativa dei dati
4 June 2014 (CNR Bologna, Italy)

Giuseppe Fiameni: Accesso Aperto ai risultati della ricerca dal punto di vista del CINECA: Pratiche correnti, Sfide e Piani futuri
Open Science 2020 - Harmonizing Current OA practices with H2020 Guidelines, 8 April 2014 - ISTI CNR Pisa, Italy

Giuseppe Fiameni: Towards a data science infrastructure
ESP Symposium, ICTP Trieste 13-14 November 2014

Giuseppe Fiameni: A HPC infrastructure for processing and visualizing neuro-anatomical images obtained by Confocal Light Sheet Microscopy
HPCS 2014, 21-25 July, 2014 (Bologna, Italy)

Giuseppe Fiameni: e-Infrastructure Commons, data management, user aspects, and future e-Infrastructures
Open e-IRG Workshop, 9-10 June 2014 (Athens)

Lectures

Giovanni Erbacci: Supercomputers, models, and simulation: a bridge between basic science and neurosciences
Workshop 'Dagli Atomi al Cervello',
27 January 2014(Milano, Italy)

Giovanni Erbacci: An European HPC Infrastructure for computational Sciences
ICT@INAF Workshop,
16-19 September 2014 (Pula, Sardinia)

Tutorials

Fabio Affinito, Francesco Salvadore
Intel Xeon Phi programming models
HPCS 2014, 21-25 July, 2014 (Bologna, Italy)

Claudio Arlandini, R. Vadori: Design improvement of a rotary turbine supply chamber through CFD analysis
PRACEdays14

Paolo Cavallo, Claudio Arlandini: HPC application to improve the comprehension of ballistic impacts behaviour on composite materials
PRACEdays14

Claudio Arlandini
Fostering Technological Innovation in Industry: Challenges and Opportunities
USE SCIENCE Conference, Riga Technical University (RTU)
28-29 November 2013

Presentations

Giuseppe Fiameni: New Opportunities in High Performance Data Analytics (HPDA) and High Performance Computing (HPC)
HPCS 2014, 21-25 July, 2014 (Bologna, Italy)

Giovanni Erbacci: The SHAPE Programme for Competitive SMEs in Europe
PRACEdays14

Giovanni Erbacci: PRACE and the HPC services for Industry
ISC'14, PRACE booth, June 2014

Massimiliano Guarrrasi: Infrastruttura HPC CINECA
Unipa ed il calcolo ad alte prestazioni: Incontro con il CINECA, 26 June 2014

Fabio Affinito: Quantum Espresso developers' meeting
January 2014, Lausanne (CH)

Fabio Affinito: Intel EMEA IPCC roundtable
April 2014, Cambridge (UK)

Fabio Affinito: European Intel IPCC meeting
September 2014, Berlin (D)

Giuseppe Fiameni: Special Session on Big Data Principles, Architectures & Applications (BDAA 2014)
HPCS 2014, 21-25 July, 2014 (Bologna, Italy)

Publications

M. Guarrasi, N. Li, S. Frigio, A. Emerson, G. Erbacci
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Awards

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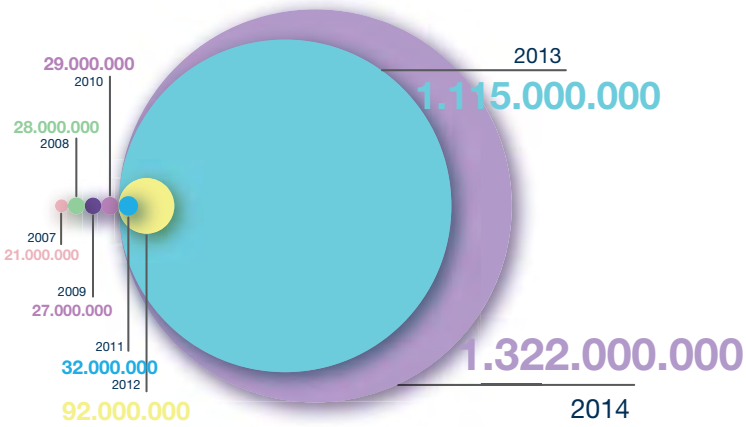
Our scientific support, users, impact

The mission of Cineca is to offer support to the research activities of the scientific community through supercomputing and its applications. It offers leading-edge computational resources and specialized personnel highly qualified for assisting researchers in the use of the technological infrastructure.
Our registered users are 2089 (as October 2014); 1689 (80,9%) of them are active users (with an associated research grant).
Among the active users, 1370 are males (81%) and only 319 females (19%), the mean age is 38, while the youngest user is 20 years old and the oldest is 81. 80% of the users have an affiliation with an Italian organization and the remaining 20% with a foreign institution (see Figure 1). In Figure 2 is reported the classification of the user Institutions. More than 90% of the users belong to public or no-profit bodies in the research environment, 60% to Italian Universities, 15% to foreign Universities, 10% to the National Research Council, CNR.
PRACE, ISCRA and LISA are the three grant allocation frameworks, strictly based on a peer-review system with two calls per years. Through this allocation schema scientists and engineers can gain access to the most advanced computational resources and services for scientific discovery. In Figure 5 the core-hours exploitation in 2014 is reported.
Cineca puts a strong effort in the support of its users.
The figures for 2014 are as follows:

- 2759 contacts were received: 763 reporting problems, 872 for service requests and 1061 for information requests. The average time spent for taking the request into account is less than one hour, with a decreasing trend with respect to time (0,75 hours in January and 0,44 hours in October 2014);
- a number of scientific applications and libraries are installed by the staff and made available to all users. Sometimes, due to specific obligations by the software vendors, the user must acquire a personal license; in any case the application is pre-installed and available on the HPC platform. All available applications and libraries are described on the web site (hpc.cineca.it/content/software). They cover several scientific fields: Chemistry, Physics, Life Science, Engineering, Astrophysics; as well as scientific visualization, mathematical and I/O libraries. At present about 55 applications and libraries are available on one or more HPC platforms in Cineca.

In summer 2014 Cineca conducted a survey to measure the user satisfaction regarding the HPC help-desk service. A total of 152 answers were collected, showing high satisfaction levels: in the range from 1 (lowest) to 5 (highest) the average mark is 3.9, with a peak of 4.3 related to competence and courtesy and a lower value of 3.4 for the on-line documentation (the whole survey is available on www.hpc.cineca.it/content/survey-results).
The impact of the HPC service offered by Cineca on the scientific communities and on innovation at large is pointed out by information extracted from the reference database “Web of Knowledge”. By analyzing the publications using HPC technologies in all the science and engineering fields, on a five years time-span (2009-2014), we got 2073 publications mentioning Cineca as funding agency.
97% of all publications have at least one author from an Italian organization. Among the authors coming from foreign countries, the largest part comes from USA (15%), then Germany (14%), France (14%), Spain (9%) and England (7%), followed by Switzerland, Netherlands, Japan, etc.
In Figures 3 and 4 are respectively reported the Journals where the researchers published most frequently and the main research areas of the publications.

Elda Rossi, Claudia Truini
Cineca



Scientific computing core hours production

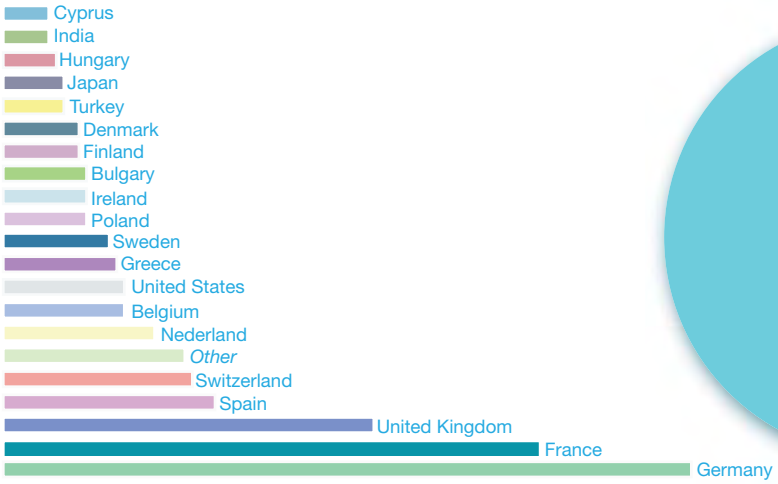


Figure 1: Cineca users with affiliation to foreign entities.

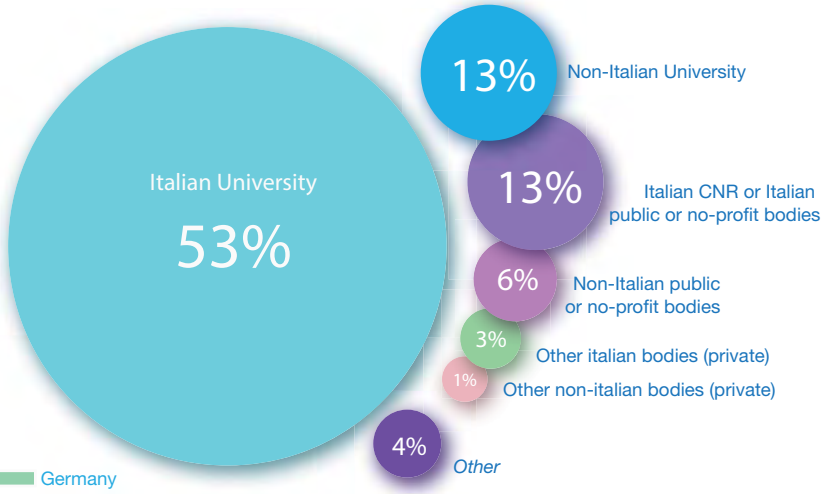


Figure 2: Classification users institutes.

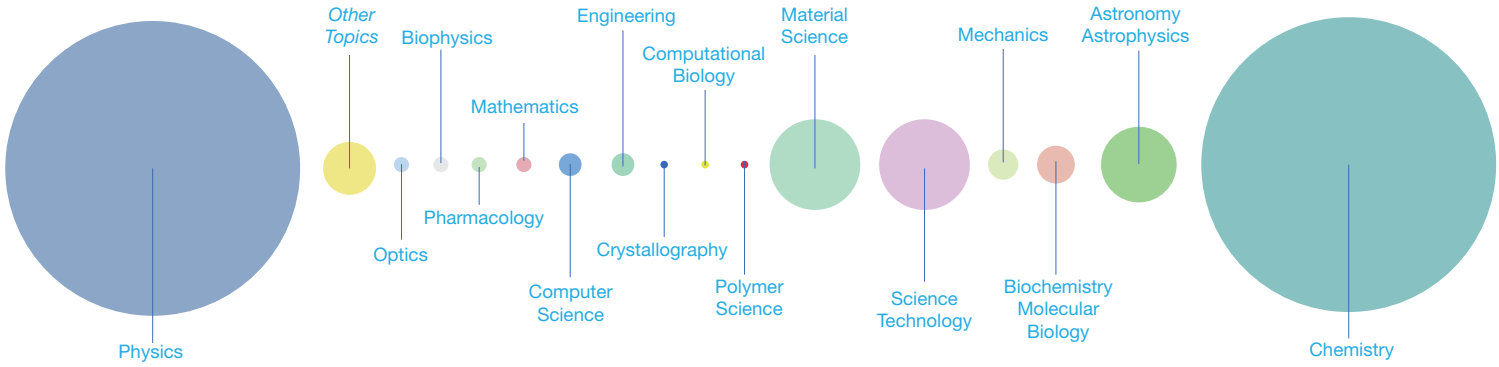


Figure 3: Research Areas of the publications mentioning Cineca (%).

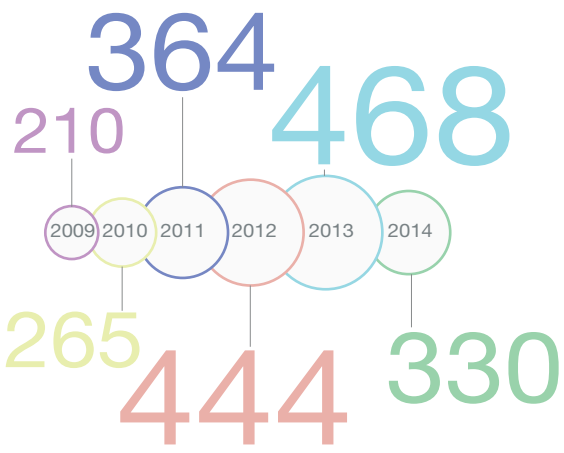


Figure 4: Total number of publications from year 2009 to 2014.

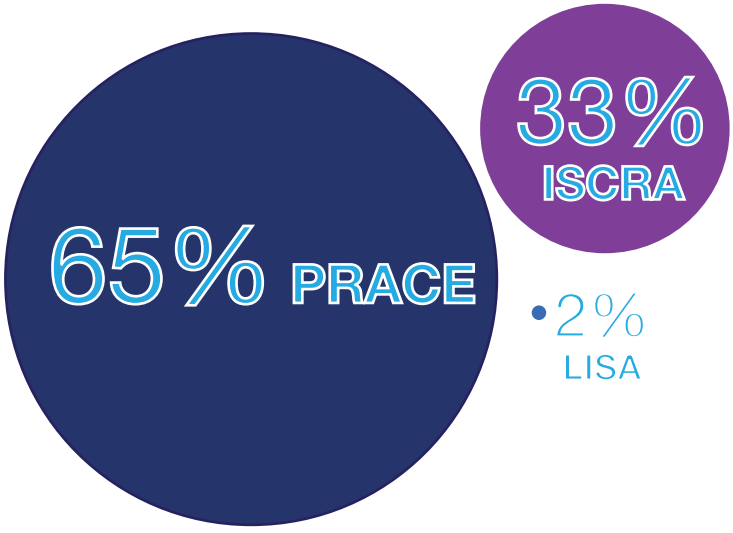


Figure 5: One billion Core Hours allocated on HPC infrastructure via call PRACE, ISCRA, LISA (%).

Research and Development as part of our structural capital

The idea of HPC being a leading-edge niche and just the narrow pinnacle of the performance pyramid misses the real point of HPC. It implies that the hardware is the only dominating factor. In reality High Performance Computing is really much more than just a High Performance Computer.
This works two ways: powerful hardware alone won't be sufficiently enabling for advancing science and knowledge (apart from few fortunate use-cases); and a real step ahead can be also achieved without extreme leading hardware.
Powerful hardware is one ingredient, but equally important are other performance contributions: software applications, support to the software infrastructure, expertise and skills of HPC personnel, advanced user support and enabling consultancy, business processes and R&D activities, as a very valuable, even if intangible, outcome of all the previous performance contributors. A successful high performance computing infrastructure and service requires a well-rounded ecosystem and a good team, which maintain persistent its development process.
This is the main reason for a number of continuous activities related to Research and Development both by means of participation in several projects funded at the European level, and at the Italian level by means of flagship and national actions (this is particularly noteworthy because of highly competitive and very selective calls), and by activating internal development projects to cover needs that are not addressed by any other opportunity.
Some activities belong to the European project landscape: the actions regarding the development of the infrastructure service provision like PRACE and EUDAT; the co-design actions toward exascale like the Montblanc and Deep technological projects; vertical scientific challenges like Human Brain Project; the support of the innovation process of industry, particularly the small and medium ones, like the Fortissimo project. Other activities refer to national advancement like Epigen and Nexdata projects, and finally some activities have the objective to cover a strategic vision like the internal funded "big data" project.
The reported panorama of the current Research and Development projects in progress provides a complete picture about this valuable activity, which has three main outcomes:
• the technological coverage of the HPC domain, that is characterized by a very fast innovation process;
• the continuous improvement of the level of know-how held by the Department;
• a very effective way to improve the skills of the human capital on board of the Department, which is a key factor for the persistency of our action for the benefit of our stakeholders' basis.
In the end we, as the SCAI Department, are driven by really big, really fascinating, and really difficult science applications that demand big machines. With big science as our strongest motivator, the HPC community continues to seek out ways to unravel longstanding scientific mysteries and find new opportunities for scientific discovery using our current and future systems. And that is a big challenge that is worth pursuing.

Giovanni Erbacci
Cineca

International collaborations

Cineca's role as leading HPC center is not only prominent in the Italian scientific and research landscape but it has reached an international dimension. Since its constitution and for the last 44 years the HPC department of Cineca has been active internationally where similar organizations have been working for the deployment of generations of leading edge systems and for the provision of highly efficient services.
Our international collaborations take an array of different forms and follow the path indicated by the EC strategy on HPC presented in the document "HPC: the Europe's place in the global race", published in 2012. In that document the basic pillars of the EU strategy are identified as: Infrastructure, Technology, Applications.
Cineca plays a key role in the PRACE Association (Partnership for Advanced Computing in Europe), the pan-European HPC infrastructure. it is one of the four hosting members that are the top of the HPC ecosystem in Europe. In that role Cineca has contributed more than 2 Billion core/hours to the European scientific and research community on its large-scale FERMI Blue Gene/Q system. Cineca is also serving as Chair of the PRACE Council and as member of the Board of Directors.
On the side of the technology pillar, Cineca is one of the 'Founding Fathers' of the European Technology Platform (ETP4HPC). The vision and mission of the ETP is rather wide for what concerns the impact on the industrial components of the HPC ecosystem. However the ETP aims also to leverage the transformative power of HPC in order to boost European competitiveness in science and business, to foster joint initiatives among ETP members and other stakeholders in the area of research and innovation programs. A relevant achievement of the ETP is a Contractual Public-Private Partnership for European High-Performance Computing with the European Commission. Cineca is member of the ETP Steering Board as one of the representatives of the computing centers that are members of the ETP.
A further collaboration opportunity is represented by the Memorandum of Understanding among four of the top centers of the European HPC ecosystem: Barcelona Supercomputing Center (BSC), Cineca Consorzio interuniversitario (Cineca), Commissariat à l'énergie atomique et aux énergies alternatives (CEA) and Forschungszentrum Jülich (FZJ). They have agreed to coordinate themselves in order to continue the implementation of the European High Performance Computing (HPC) strategy through technology development as proposed in Horizon 2020. The objectives of the agreement are to coordinate HPC R&D and Innovation efforts of the partners, leveraging joint efforts for better effectiveness; to help building a globally competitive value chain and HPC flagship industry from hardware to applications; to support the EU HPC strategy defined at the level of the European Commission.
As far as the applications pillar is concerned, Cineca is actively participating to a number of preliminary initiatives aimed to establish the so-called Centers of Excellence. The Centers of Excellence are expected to be the place where R&D is performed at world standard enabling technological innovation and potentially becoming essential for endogenous economic growth as well as to attract private investments.
Last but not least Cineca is leading a joint international effort for the first European Pre-Commercial Procurement (PCP) in the area of HPC systems. The joint procurement is a cross border collaboration among five partners of the third PRACE Implementation project (PRACE 3IP). The procurement is expected to end in 2017 with the deployment of a small scale production system implementing innovative technologies for energy efficient HPC machines.

Sergio Bernardi
Cineca

You may have seen us around ...

12 months full of events…
We are proud to have been present in some of our field's best events worldwide and to have hosted some important events in Italy featuring outstanding key-players in HPC.
After the first experience, which we found very positive, in Salt Lake City in 2012, even 12 months ago we decided to be present at SuperComputing with our own Cineca booth, to tell our friends and followers one year of work and innovations in terms of services offered, collaborations activated and results obtained. The presence at the SC conference in Denver in 2013 gave important numbers in terms of contacts at our booth, going from about 550 in 2012 to more than 700, with some relevant opportunities of new collaboration and with evident improvement in spreading the awareness of our activity as Italian and European HPC infrastructure in support of the scientific community.
With the aim of increasing the fundamental involvement of the research community in our activities and to incorporate and expand knowledge, perspectives and resources that each player brings the ecosystem, we faced 2014 with increasing energy and attention towards more networking opportunities and "exposure".
For the first time we were present with a small booth Cineca the European edition of SuperComputing, ISC14, in Leipzig, with a considerable number of contacts (compared to the overall number of participants, less than the American version) and a strong networking action (especially effective occasion at that time of the year, coinciding with the calls for proposals issues by the European Commission in Horizon2020). We were back to the scene in November 2014 at SuperComputing with a large booth, in collaboration with INFN, the National Institute of Nuclear Physics and the aim of presenting the Italian house of high performance, involving the major research institutes acting in intensive computing, throughput computing and data analytics, working together towards the idea of buiilding up the national cyberinfrastructure.
This new integrated arrangement of national infrastructures has given excellent results in terms of visibility (about 1000 contacts in the 4 days of the exhibition) and we are hopeful in terms of future collaborations and reinforcement of the existing links, Europeand and worldwide.
July was a full and extremely important month, thanks to the opportunity that we had to host the conference "HPC & Simulation", sponsored by IEEE, welcomed by Professor Braga, Vice-Chancellor of the University of Bologna. 300 experts from all over the world met in Bologna, for the five-day conference, between July 21 and 25, 2014 with the aim of addressing, exploring and exchanging information on the state-of-the-art in high performance and large scale computing systems, their use in modeling and simulation, their design, performance and use, and their impact.
Second important appointment will be the December 5 workshop, "PICO: the Cineca solutions for Big Data Science". Cineca has recently initiated a new programme for the promotion of Big Data Science, addressing the challenges that arise when either the data volume, structure or the speed of collection, make processing difficult. A new computing system, named PICO, was installed at Cineca. PICO is intended to enable new BigData classes of applications, related to the management and processing of large quantities of data, coming from both simulations and experiments. There will be a particular focus on all emerging scenarios which require an interactive model (Urgent Computing), as well as new paradigms of resource utilization through Cloud Computing technology.
PICO will be officially presented in a public workshop and experts in different disciplines will show how PICO can effectively help them to solve their problems of BigData management.

Francesca Garofalo
Cineca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Improving opportunities for research and scholarship: building of a new generation of HPC

The concept of the "knowledge economy" means a new phase of development in which scientific knowledge and human resources are strategic growth factors and in which it is evident a close connection between the processes of learning, innovation and economic competitiveness [1].

A cloud of people, researchers, students, scientists and engineers attended the HPC department over the past 12 months, with different forms of internship, attendance and cooperation, but in all cases, creating interesting situations of mutual exchange and enrichment and broadening the perspectives of future collaborations.

Increasing attention has been paid, in the last year here Cineca, on the creation and dissemination of knowledge in the field of HPC: selecting and training the most promising scientists and attracting researchers and practicioners for fostering future interdisciplinary cooperation were two strong goals that we have set as priorities.

Training has always been a hallmark of the support activities carried out by Cineca to the Italian research community and users, extended from 2012 to the European researchers, being Cineca recognized as PRACE Advanced Training Centre in HPC.

In total during 2014 we reached quite impressive numbers:

15 courses, distributed in 29 different editions distributed in three locations of operation of the consortium, 3 schools in 6 editions.

In addition, teaching collaborations have been turned on into 6 academic courses (Masters, Doctorate schools, specialist schools, workshops), held in some universities. 50 people in the SCAI department contributed as teachers, for a total of 150 days of lectures and highly specialized training.

In total, at 31 October 2014 over 610 Italian and European researchers benefited of the Cineca training programme and by the end of the year students will exceed abundantly the amount of 700, increasing the 2013 figures by a 10%.

Besides traditional lectures, many other initiatives attracted very young promising scientists to Cineca, to spend short or extended period of visits under the mentoring action of our experts, who help them to maximize the output of their research in approaching or deepening their expertise in HPC techniques.

The attendance of the training events often gives rise to long-lasting partnerships. One of the 2014 cases is Eric Pascolo, University of Modena, who is playing his master thesis supported daily by a Cineca expert, which is accompanying him in his career; some interesting job prospectives already opened up for Eric at an outstanding national research institute.

Summer of HPC (https://summerofhpc.prace-ri.eu), a PRACE initiative, is a fascinating exemple of collaboration experience: a couple of young scientists, in 2014 Vojtech Nikl and Konstantina Lazaridou, selected on the basis of the topic proposed, spent at Cineca in Bologna two months in summer, working on data visualization techniques applied to coronal loops on the shell of the sun and wind tunnel turbulences, living in our guest-house and sharing our office and habits.

Another pleasant contribution of SCAI in the mission of building a new generation of HPC was the collaboration with Mustafa Tokgöz, a young guy from Turkey concluding his studies at Gdansk University of Technology in Poland. Mustafa applied for an internship for a long summer period and was amazingly involved in the user support experts day-by-day activity, gaining a rich experience and creating links for possible long-lasting research collaborations.

As part of a framework agreement between Cineca and the University of Bologna, a close and still ongoing collaboration has been created between a group of seven engineers of the Department of Electrical and Information Engineering of Energy and the Department of Computer Science and Engineering and a number of specialists in SCAI: objective is to develop advanced techniques of thermal control and energy for the minimization of the cost of operating the apparatus of supercomputing subject to constraints of quality of service.

Other collaborations are ongoing in the pharmaceutical field, to develop advanced techniques for multiscale simulations of ion channels phones for the discovery of new potential drugs and in the field of processing of data streams of large size, for developing advanced techniques of treatment, storage and processing of big data and data stream scenarios for Smart Cities.

(1) (translated from "Le reti di conoscenza e innovazione e il knowledge management territoriale", Riccardo Cappellin, published in Innovazione, sviluppo e apprendimento nelle regioni dell'Europa mediterranea, Franco Angeli, Milano, 2003).

Francesca Garofalo
Cineca

Stage

During my Master Thesis in Applied Physics I spent a year and a half in the HPC department of Cineca. In this period I worked with Carlo Cavazzoni on the Quantum EXPRESSO package, one of the most highly optimized HPC applications that has been developed. Working in Cineca, side-by-side with HPC experts, gave a professional imprint to my training – up to then it was mainly scientific and I wouldn't have been able to obtain this kind of preparation by just attending university. It has been a sort of internship to me: I started as a newbie, knowing very little in this field , but I learnt how to develop software working in close collaboration with Carlo. The more I worked alongside Cineca's HPC team, the more I was able to understand different hardware and software problems involved in HPC. The team itself is very close-knit, and it was very helpful in every aspect of my work. Working in the HPC department of Cineca and attending the centre's courses gave me the opportunity to meet many national and international experts, who were collaborating with Cineca on many projects. I was also able to directly see how a Computer Centre works and to understand how many scientific and technologic fields unite in order to be able to provide the most advanced computing resources. I was surprised to meet in this world many professionals with backgrounds very far from IT. My personal programming skills advanced remarkably, since I needed to learn how to work on software that had to be extremely performing, running on computers with unique and extremely complex architectures. Thus, I learnt that the software developer's main task is to write a machine-specific code, in order to exploit every single FLOP. Moreover, thanks to the period I spent in Cineca I could join the International Master Programme in HPC by SISSA and ICTP, which I am attending now. If you are a student and you are searching for a thesis, I suggest you to spend a period in Cineca's HPC department – especially if you like this field, or if you want to find out more about it. You will find a dynamic and stimulating environment, where you will be able to work on the newest technologies available on the market, on projects to develop new machines or on the optimization and the innovation of the existing computers.

Eric Pascolo
Bologna University

50 teachers

150 days of lectures

700 post-graduated students

15 courses
3 schools
29 editions
6 editions

3 masters
2 doctorate schools
CINI
La Sapienza
Politecnico Milano
OGS
SISSA-ICTP

10 internships
2 undergraduates
4 master thesis
4 PhD

Summer of HPC 2014

Hello, my name is Vojtech Nikl and I come from the Czech Republic. Earlier in 2014, I was selected to participate in the Summer of HPC 2014 programm. During July and August I was working at Cineca Supercomputing Center. My main goal was to visualize the results of scientific experiments and measurements, namely coronal loops and wind tunnel turbulences. The visualization process consisted of data filtering, data representation, animation over each time step and video editing.

I worked mainly on the PLX cluster and its RVN nodes, which support remote visualization through remote displays. This is very useful because it is possible to work from home over the internet. However I spent most of the time working directly at Cineca since there is a great working environment and a team of HPC professionals who are ready and happy to help anytime.

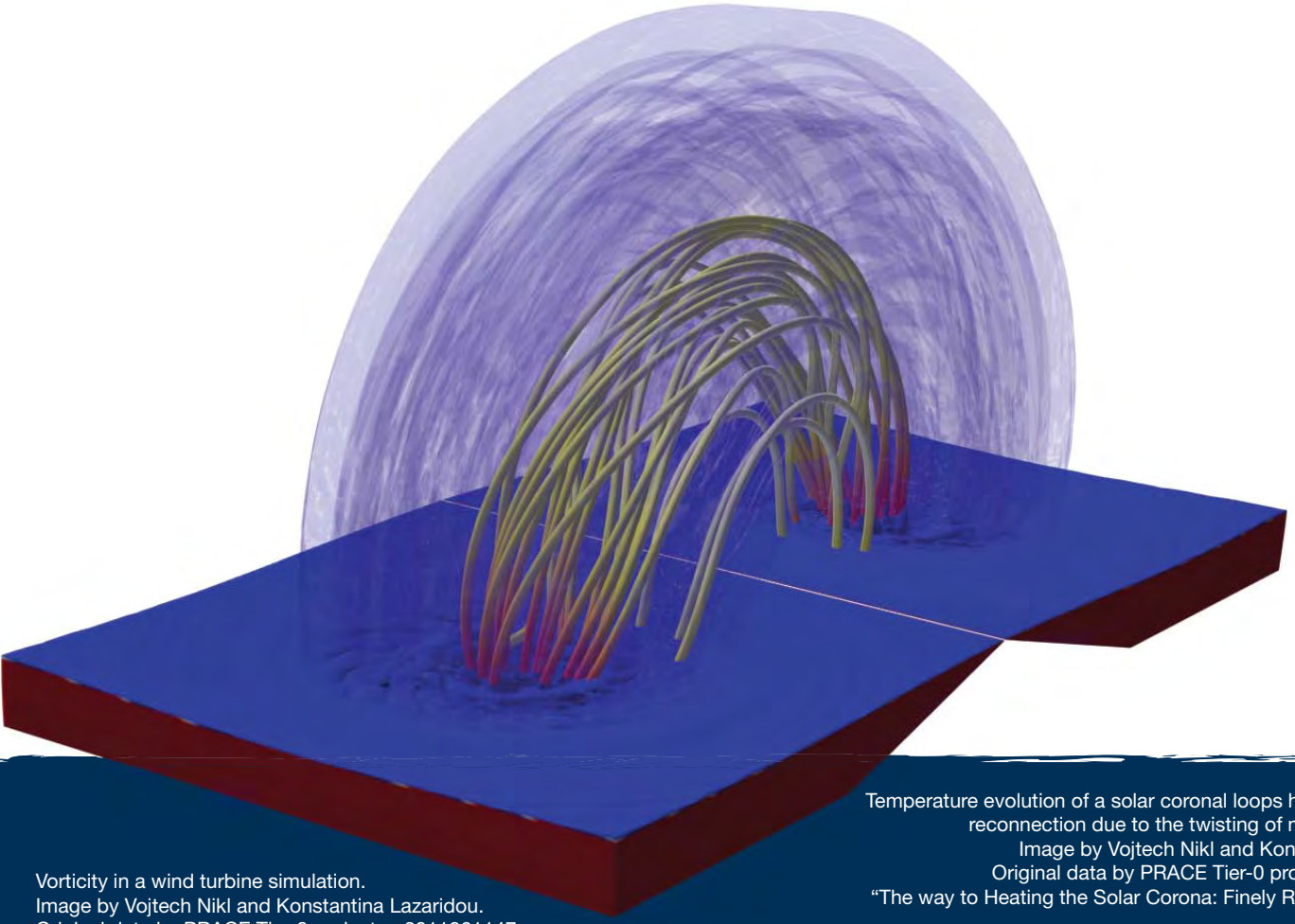
Besides the visualization itself, Cineca allowed me to use their biggest cluster, Fermi (over 160 thousand cores), to test my master's thesis program, which deals with the hybrid MPI/OpenMP implementation of the Fast Fourier transform in the k-Wave project. All the support from Cineca to young scientists like myself is really invaluable.

I was accommodated in one of the Cineca's apartments for international guests. Both the apartment and the location are very beautiful; about 15 minutes walk from Cineca. The accomodation, flight tickets and the whole stay in Italy was fully financially supported by PRACE via schollarship.

The two months passed by very quickly. I miss the supercomputers and passing by them every morning and afternoon. Cineca even allowed me to visit the machine room and take a look at the computers up close – another unforgettable moment. All together, I have converted over 250GB of data into a single 20 min FullHD video using over 70 thousand core hours. It was very time demanding and sometimes exhausting work, yet it was well worth it. One of the Cineca's universal instructions "In the case of panic, keep calm and use the default" always cheered me up. However, the most helpful were the people themselves, who were ready and happy to help any time. I would like to thank especially my supervisor and tutor, Dr. Massimiliano Guarassi, without whom the final result would not have been possible to achieve.

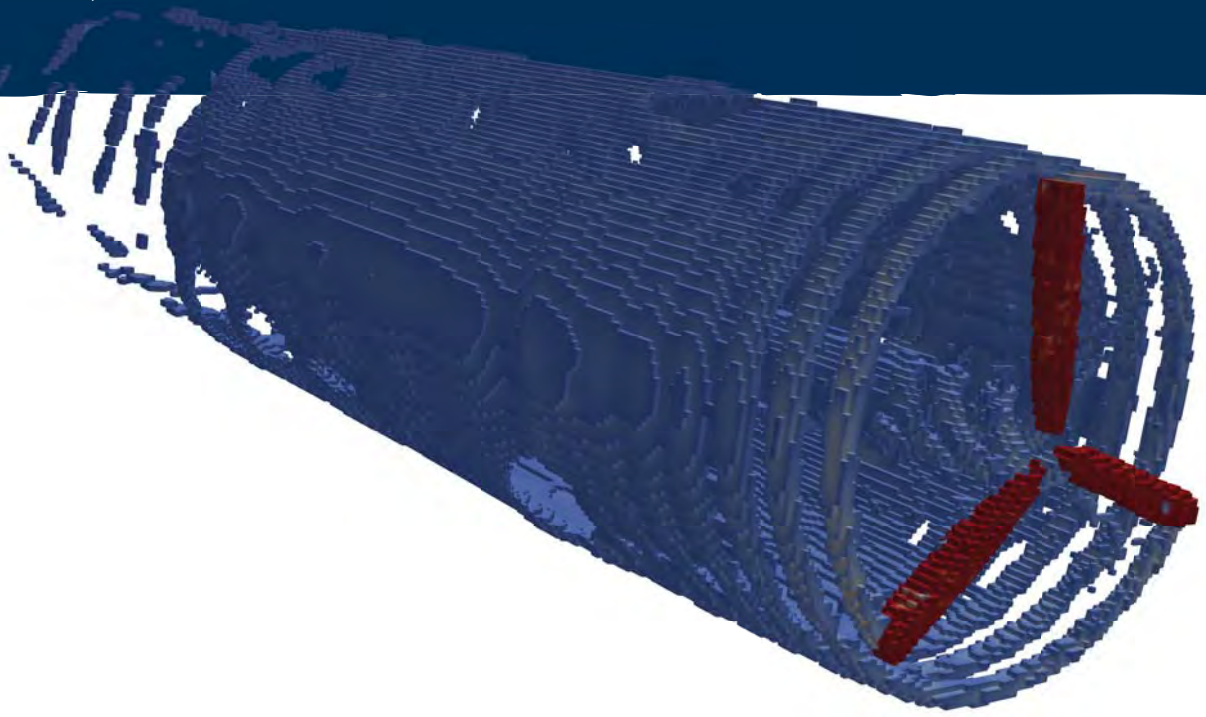
Even though I had been a little bit afraid before coming to a foreign country completely on my own, it was the best summer I have ever experienced. The Summer of HPC was definitely a life changing experience for me and I wish I could repeat this sometime in the future. I gained a lot of insight about how the whole HPC infrastructure works, how to use the resources properly and responsibly and how to properly visualize a set of scientific data. I thank PRACE and everybody involved very much for this awesome opportunity and I hope this is not the last time we cooperate together.

Vojtech Nikl
Brno University of Technology



Temperature evolution of a solar coronal loops heated by magnetic reconnection due to the twisting of magnetic field lines.
Image by Vojtech Nikl and Konstantina Lazaridou.
Original data by PRACE Tier-0 project n.2011050755
"The way to Heating the Solar Corona: Finely Resolved Twisting of Magnetic Loops"
F. Reale, S. Orlando, M. Guarrasi, M. Miceli

Vorticity in a wind turbine simulation.
Image by Vojtech Nikl and Konstantina Lazaridou.
Original data by PRACE Tier-0 project n. 2011061147
"Innovative Computational Methods for Wind Farms"
P. Schito, R. Ponzini, A. Invernizzi, A. Zasso, C. Gorlè



The case of Quantum ESPRESSO community code

Material Science is one of the areas where computational science and the advent of more and more powerful supercomputers can have a large impact on science and technologies, due to the possibility to find approximate solutions of the fundamental quantum mechanical equation governing the behaviour of materials at atomic scale, for larger and larger atomic systems and with an higher degree of accurancy, shortening the path from theoretical results and technological applications, and opening up the possibility to design new materials from scratch.

Quantum ESPRESSO is a suite of codes implementing the algorithms to solve this equation and one of the most used in the high-end HPC center all around the world.

Since its official kick-off, held in summer 2002 in Princeton, Cineca is one of the main protagonist of the development and promotion of the Quantum ESPRESSO community code project, and today is a member of the Quantum ESPRESSO Fundation.

This experience represents a successful story of collaboration between computational scientists, HPC experts and the user community, allowing the suite of codes maintained by the project becoming one of the most successful world wide.

One of the key ingredient of this success is the collaboration on the code design, Cineca is responsible of what concern the parallelization, technology innovation and HPC enabling, while the scientific institution may stay focussed on the development of the science.

Another important ingredient is the joint dissemination activities, where scientists and HPC experts teach people not only about science but also about how to take advantage of supercomputers.

In fact, in many cases, the barrier represented by the stack of competences required to use high-end HPC infrastructure prevents scientists to use and exploit them.

The importance of Quantum ESPRESSO for the user community is testified by the large number of projects running on Fermi flagship system and the large share of the overall computational workload this user community has gained.

Besides supporting its user the involvement of Cineca in the Quantum ESPRESSO project has also a positive economical impact, mainly due to the EU projects where Quantum ESPRESSO represents an asset of Cineca, and in the contract that Cineca has signed with Intel to promote the development of Quantum ESPRESSO on next generation Intel microprocessor, within the Intel Parallel Computing Center (IPCC).

The interest of Intel is dual, on one side they want to ensure that Quantum ESPRESSO and its user community could exploit the new architectures, on the other side Intel itself is using Quantum ESPRESSO for its internal evaluation and Material Science R&D.

Carlo Cavazzoni
Cineca

Intel Parallel Computing Center (IPCC)

Since October 2013, Cineca has been appointed as Intel® Parallel Computing Centers (IPCC). IPCC are universities, institutions, and labs that are leaders in their field, focusing on modernizing applications to increase parallelism and scalability through optimizations that leverage cores, caches, threads, and vector capabilities of microprocessors and coprocessors. Systems in the next decade will support millions of processor cores with thousands of threads. But increased compute power will only get us so far. Future performance gains will also come through parallelism, and modernizing key applications will help us making the next leap in discovery. Code modernization is expected to enable large performance increases while maintaining the code portability that users expect.

The first target of Cineca as Intel® Parallel Computing Centers (IPCC) is the porting on the Intel® Xeon Phi platform of three codes of large interest for the Italian scientific community.

The Intel® Xeon Phi coprocessor is a platform based on the x86 architecture that features 61 cores and h 512-bit SIMD vectorial registers. The Xeon Phi co-processor that can be used both as an “accelerator” when coupled to a host processor and as a independent computing unit. The main advantage of this co-processor is that “classical” programming paradigms, such as MPI and OpenMP, can be used to exploit its computational power. In addition, the work necessary for porting a code on the Xeon Phi results in a modernization of the whole code whose benefits will be available for any kind of other platforms.

For the first year of activity as IPCC, three codes have been selected: Quantum Espresso, SpecFEM3D and Yambo.

Quantum ESPRESSO (opEn Source Package for Research in Electronic Structure, Simulation and Optimization) is an integrated suite of computer codes for electronic-structure calculations and materials modeling, based on density-functional theory, plane waves, and pseudopotentials. It is freely available to researchers and widely adopted from both from the Italian and the international scientific community. Quantum ESPRESSO builds upon newly restructured electronic-structure codes that have been developed and tested by some of the original authors of novel electronic-structure algorithms and applied in the last twenty years by some of the leading materials modeling groups worldwide. Innovation and efficiency are still its main focus, with special attention paid to massively parallel architectures, and a great effort being devoted to user friendliness.

SPECFEM3D Cartesian is a community code that simulates acoustic (fluid), elastic (solid), coupled acoustic/elastic, poroelastic or seismic wave propagation in any type of conforming mesh of hexahedra (structured or not). It can, for instance, model seismic waves propagating in sedimentary basins or any other regional geological model following earthquakes. It can also be used for non-destructive testing or for ocean acoustics. SPECFEM3D is a code adopted by the italian geophysical community and by the INGV researchers.

YAMBO (Yet Another Many Body cOde) is a is a code for Many-Body calculations in solid state and molecular physics. Yambo uses as input the wavefunctions calculated by other codes (in particular, it has an interface for Quantum ESPRESSO and Abinit codes) and can compute several properties of excited states (dielectric screening, GW approximation, Bethe-Salpeter equation). This code was originally developed at the University of Rome “Tor Vergata” and it was rapidly adopted by a large number of users in Italy and all across Europe. With the support of Cineca, this code was recently modified and made able to scale on massively parallel computers (i.e. FERMI Blue Gene/Q).

During the first year of activity we worked on the three codes reporting successful results. In some cases we encountered problems that were tackled with the precious support of the Intel® staff. This active collaboration between Intel®, Cineca and software developers was essential to perform the work and to reach the desired target: modernized codes that are ready to efficiently run on new architectures such as the new Intel® Xeon Phi coprocessors. A first step towards the next exascale challenges.

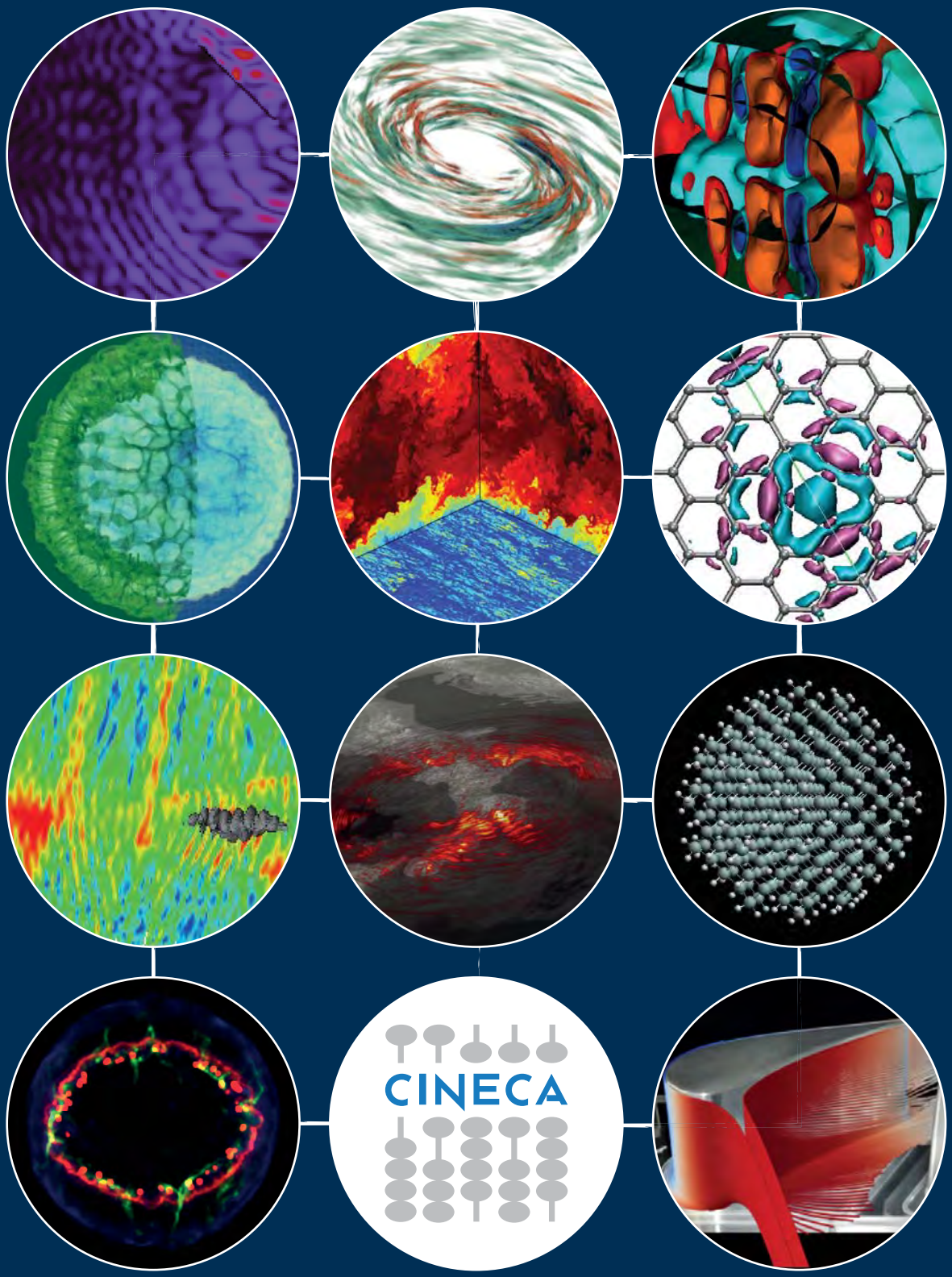
Fabio Affinito
Cineca

SPECIAL

The public goodwill intangible asset of Cineca SCAI

By definition the value of goodwill typically arises when the value amount of a company is higher then its revenue value (in example, for an acquisition, a company needs to pays more for the target company, over the target's book value usually accounts for the value of the target's goodwill).
Goodwill value is difficult to price, but it does make an entity more valuable. For example, a company like Coca-Cola (who has been around for decades, makes a wildly popular product and is generally positively perceived by the public) would have a lot of goodwill.
Of course, since the components that make up goodwill have subjective values, the assets related on are just intangible, is very difficult to define a metric to measure its value, even if in the domain of private organizations the substantial risk of the goodwill is accounted as a risk of investment, as any others strategic development decision.
For an institution which has a very clear statutory mission, as the one for the research and innovation enabling support related to SCAI, the goodwill value is typically valorized answering to the following (simplified) question: what about with or without Cineca HPC action?
The way to answer the previous question has to be anyhow depurated by the obvious points referring to the physiological outcome assigned to our role, as providing service for access to high performance computing and the most advanced digital infrastructure for science in Italy, support the development of the stakeholders ecosystem, managing the business model that makes most effective the utilization of the available economical resources.
With such a rationale as criteria to render the public goodwill of the value of Cineca, in the following will be highlighted some examples, which better provide sense of goodwill of the value of Cineca.
The first enabling service is represented by the operational service for the numerical weather forecast for the National Civil Protection, under the supervision of the Meteorological service of the Emilia Romagna Region. Such a service is a service for value, but at the same time it is clear that Cineca will never discontinue the service if not interrupted by the contractors. The matter of the economical sustainability cannot be disregarded, but Cineca is committed for its best for a service which represents a potential value at socio-economical level.
The second action presented regards the participation of Cineca on the construction of a digital service for a bioinformatics infrastructure for the Epigenetic research and for a personalized medicine outcome in the next future. This action leads to the support of the Italian action in the context of European Elixir project and to enable the development process in a domain which is not yet mature enough to compete as the others domains in the access to HPC service as defined by means of open access peer-reviewed processes, but is strategic again for its socio-economical impact and for the benefit that the entire public health system may receive. Cineca invested in that domain providing services to the entire national bioinformatics community and defining constituency agreements with qualified players in this context, as the charities entities, the disciplinary labs, the regional public system.
The last action has been a service provision to support the forensic investigations for extreme events, which mandatorily should count on the access to the top level national facilities. In particularly we collaborate with CNR-INSEAN the Italian Ship Model Basin for the support to the forensic investigation regarding the incident involving the Jolly Nero ship in the basin of the port of Genoa.

Sanzio Bassini
Cineca


CINECA

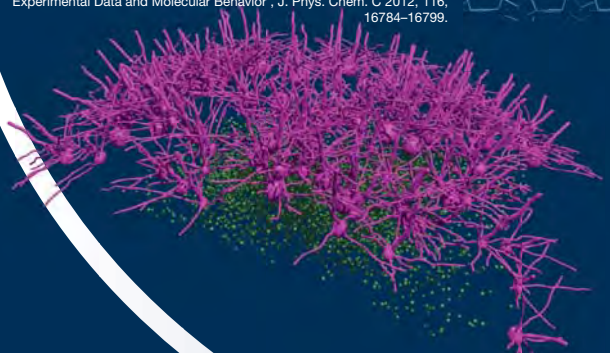
Diffusion mechanism of a dye molecule (oxonine) along the nanochannels of zeolite L.

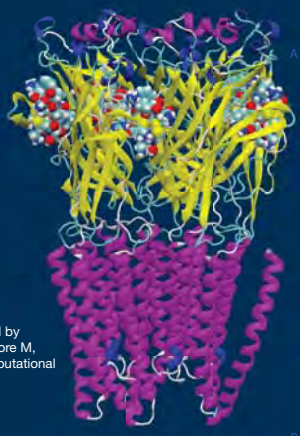
Left: the molecule is oriented perpendicular to the channel axis; with this orientation, the molecule is trapped in one cage and cannot diffuse along the channel. Right: the molecule is oriented parallel to the channel axis; with this orientation, the molecule can move from cage to cage. Middle: the transition from the perpendicular to the parallel orientation is achieved by a squid-like bending of the dye molecule.

E. Fois, G. Tabacchi, G. Calzaferri Orientation and Order of Xanthene Dyes in the One-Dimensional Channels of Zeolite L: Bridging the Gap between Experimental Data and Molecular Behavior , J. Phys. Chem. C 2012, 116, 16784–16799.

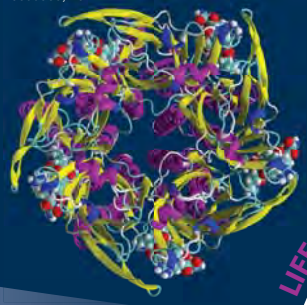
a) Depth sections of the shear velocity percentage perturbations in the 3D model of the Pacific region, obtained with the analysis of the seismological data-set.
b) Depth sections of the shear velocity percentage perturbations in the 3D model of the Pacific region, obtained with the analysis of both the seismological data-set and the gravity data-set through the parallel procedure of Sequential Integrated Inversion (Tondi et al., Computer and Geosciences, 2012).

R. Tondi, C. Cavazzoni, P. Danecek, A. Morelli, 2012. Parallel, 'large' dense matrix problems: Application to 3D sequential integrated inversion of seismological and gravity data, Computers and Geosciences, 48, 143-156.



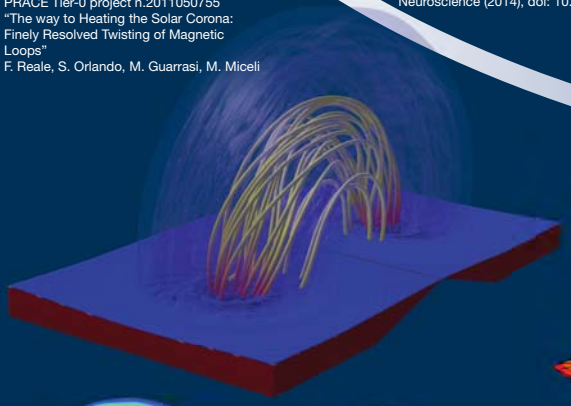


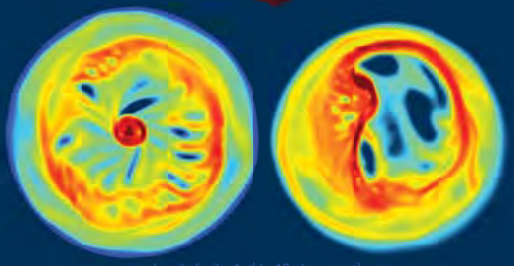
New homology model of human alpha7 nicotinic receptor generated by using the open TMD of the glutamate receptor (PDB entry: 3RIF) and the conotoxin-bound AChBP (PDB entry:2BYQ) to model the LBD. A) side view; B) top view. Conotoxin in vdw representation.
Zeynab Mohammad Hosseini Naveh,Therese E. Malliavin,Luca Maragliano, Grazia Cottone, Giovanni Ciccotti
Conformational Changes in Acetylcholine Binding Protein Investigated by Temperature Accelerated Molecular Dynamics, PLOS ONE, 9, ee88555, 2014

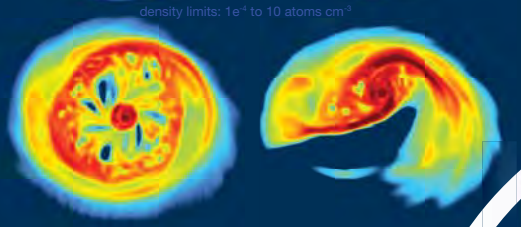


Temperature evolution of a solar coronal loops heated by magnetic reconnection due to the twisting of magnetic field lines.
PRACE Tier-0 project n.2011050755
"The way to Heating the Solar Corona: Finely Resolved Twisting of Magnetic Loops"
F. Reale, S. Orlando, M. Guarrasi, M. Miceli

"Distributed organization of a brain microcircuit analysed by three-dimensional modeling: the olfactory bulb" by Migliore M, Cavarretta F, Hines ML, Shepherd, GM Frontiers in Computational Neuroscience (2014), doi: 10.3389/fncom.2014.00050







Far field radiation pattern of a plasma antenna array
references: D.Melazzi,V.Lancellotti, "ADAMANT: a surface and volume integral-equation solver for the analysis and design of helicon plasma sources", Comp. Physics Comm., vol 185, no. 7, July 2014, pp.1914-1925

EARTH SCIENCE
LIFE SCIENCE
ASTROPHYSICS
ENGINEERING
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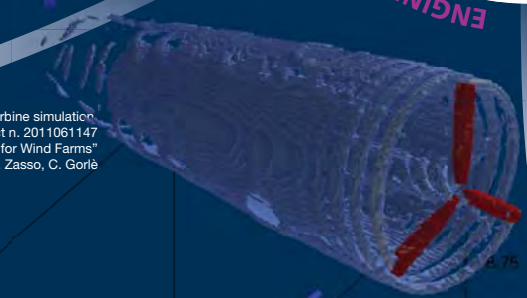
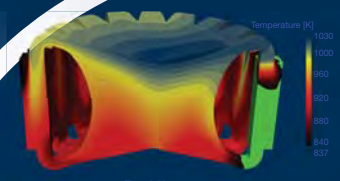
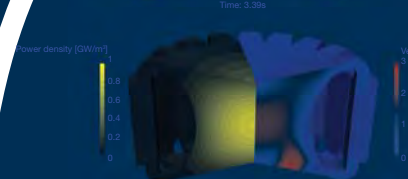
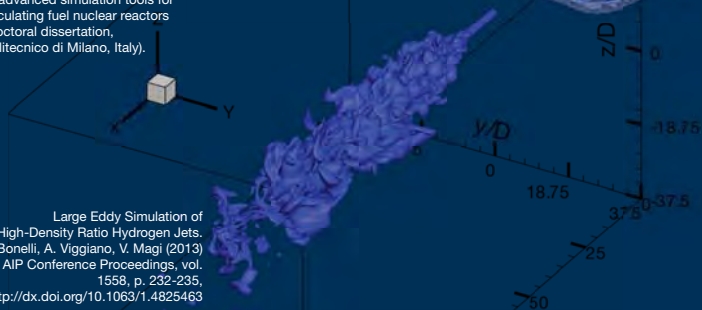


Vorticity in a wind turbine simulation
PRACE Tier-0 project n. 2011061147
"Innovative Computational Methods for Wind Farms"
P. Schito, R. Ponzini, A. Invernizzi, A. Zasso, C. Gorlè

Temperature (top), velocity and power density (bottom) fields in the MSFR after the single pump failure accident.
M. Aufiero (2014). Development of advanced simulation tools for circulating fuel nuclear reactors (Doctoral dissertation, Politecnico di Milano, Italy).



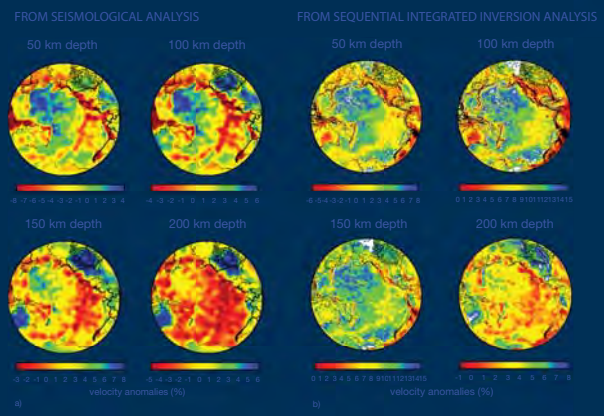


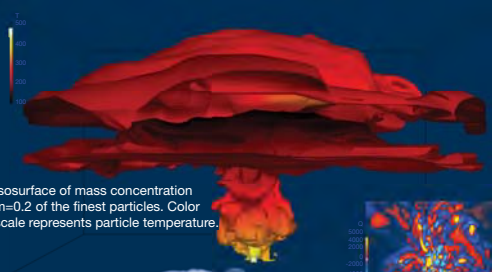


Large Eddy Simulation of High-Density Ratio Hydrogen Jets.
F. Bonelli, A. Viggiano, V. Magi (2013) AIP Conference Proceedings, vol. 1558, p. 232-235, http://dx.doi.org/10.1063/1.4825463

Collisional ring galaxies are characterized by a luminous ring of stars and gas. They are expected to form from the collision of a disc galaxy (hereafter the target galaxy) and a companion galaxy (hereafter the bullet galaxy). In the frame of the ISCRA HP10B3BJEW project, we simulated the collision between the target and the bullet galaxy by using the RAMSES adaptive mesh refinement code (Teyssier 2002, Astronomy & Astrophysics, 385, 337). We ran a large set of simulations, investigating the importance of different collision parameters (impact parameter, inclination and relative velocity). The plot shows the mass-weighted gas density map in the xy plane (i.e. the plane of the target disc) at time = 50 Myr after the collision for one of our simulations. See Fiacconi, Mapelli, Ripamonti and Colpi 2012, MNRAS, 425, 2255 for more details.

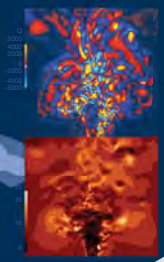
http://adsabs.harvard.edu/abs/2012MNRAS.425.2255F





Isosurface of mass concentration m=0.2 of the finest particles. Color scale represents particle temperature.

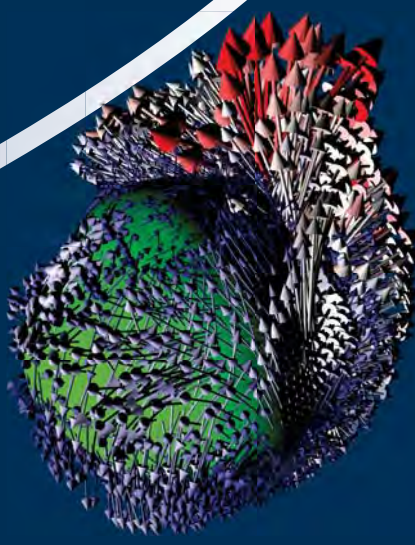
Three-dimensional numerical simulation of an eruption column in a stable atmosphere. Inflow parameters represent typical eruption conditions for a Plinian eruption (mass flow rate = 1.5 x 10^9 kg/s; exit velocity = 275 m/s; water content = 5 wt.%; temperature = 1053 K). Two particle classes of (d=0.5 mm; rho=2500 kg/m^3) and (d=15 microns; rho=2700 kg/m^3) are considered.
M. Cerminara, T. Esposti Ongaro "A fast Eulerian model for volcanic ash plumes", 2014



Distribution of the Q invariant (measuring flow vorticity) along the x-z plane across the inlet.

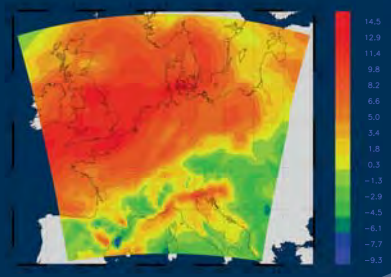
Vertical slice of mass concentration of the finest particles.

Eulerian flow acceleration A along the x-z plane across the inlet. A gives a measure of gas-particle decoupling.



Vector plot of the velocity fluctuations over the interface of the droplet (in green); high turbulence regions are shown in red, whereas low turbulence regions are shown in blue.
Scarbolo and Soldati (2013) "Turbulence modulation across the interface of a large deformable drop", J. Turbul. , 14(11) 27-43.
Scarbolo and Soldati (2014) "Wall drag modification by large deformable droplets in turbulent channel flow", Comput. & Fluids, (In Press).

Background of the zonal wind component (m/s) at 850 hPa at 12 UTC on 01 July 2012
S. Federico: Implementation of a 3D-Var system for atmospheric profiling data assimilation into the RAMS model: initial results, Atmos. Meas. Tech., 6, 3563-3576, doi:10.5194/amt-6-3563-2013, 2013.



H AND CLIMATE SCIENCE

ACE

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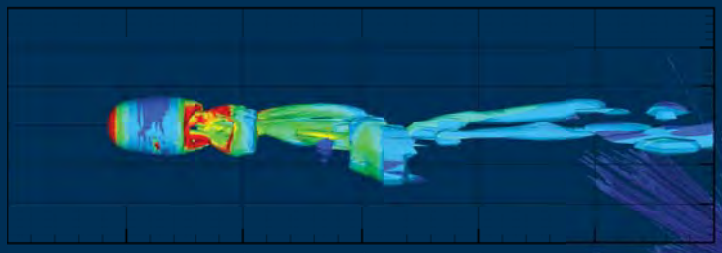
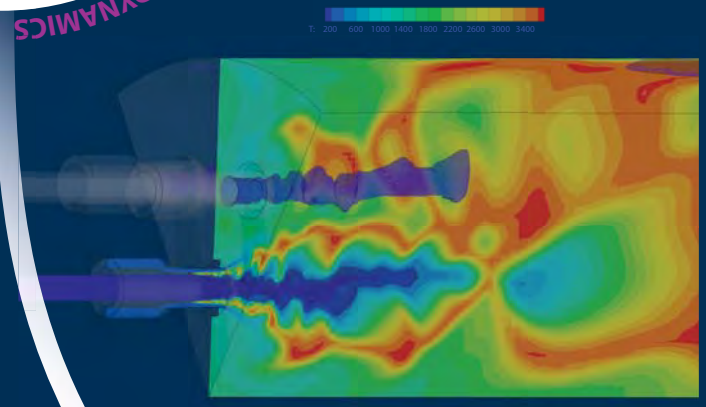
COMPUTATIONAL FLUID DYNAMICS

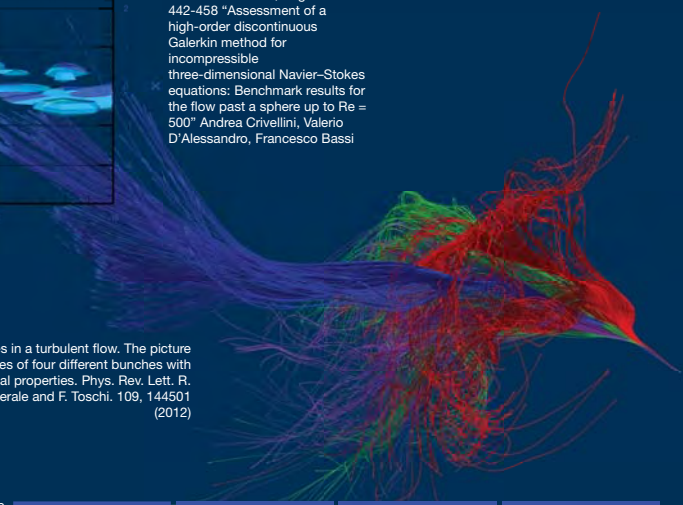


Computers & Fluids, Volume 86, 5 November 2013, Pages 442-458 "Assessment of a high-order discontinuous Galerkin method for incompressible three-dimensional Navier–Stokes equations: Benchmark results for the flow past a sphere up to Re = 500" Andrea Crivellini, Valerio D'Alessandro, Francesco Bassi



Supercritical Combustion in Liquid Rocket Engines - temperature field
Francesco Creta, Giovanna Gargiulo e Mauro Valorani

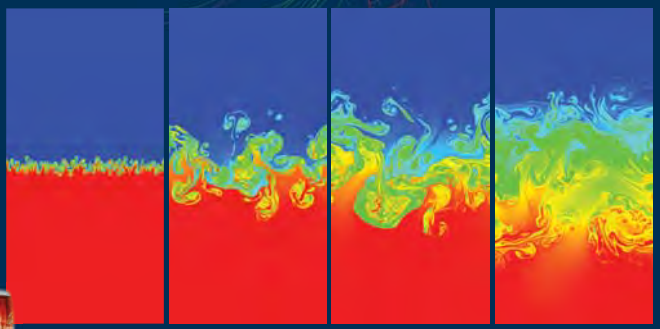
CFD Analysis of Laser-Pulse Ignition of GCH4/GO2 in M3-DLR Test Bench. M.Valorani, E.Martelli, G.Gargiulo, P.P. Ciottoli, P.Grenard J.Sender.
3rd edition of the International Conference on Space Propulsion 2012 Bordeaux, France, May 2012



Dispersion of particles in a turbulent flow. The picture shows the trajectories of four different bunches with four different inertial properties. Phys. Rev. Lett. R. Scatamacchia, L. Biferale and F. Toschi. 109, 144501 (2012)

Simulation of the Rayleigh-Taylor Instability

When a cold and dense fluid floats over a layer of warm, less dense fluid, an instability is triggered that mixes the two regions. This is known as Rayleigh-Taylor (RT) instability. This phenomenon is relevant in many areas of science and technology, from engineering to astrophysics, and its theoretical understanding is far from complete. The pictures on the right are temperature-snapshots of the time evolution of an RT instability.



This visualization uses data of a science project from a collaboration of INFN and the Universities of Ferrara, Roma "Tor Vergata", and Eindhoven.

SECTION 4

SCIENTIFIC REPORTS

Presentation of the Users' Reports

The infrastructure of Cineca is accessible according to the three specific allocation channels, PRACE, ISCRA, LISA, as detailed before or, as a residual marginal quota, to development projects and projects related to agreements of joint collaboration between Cineca and outstanding national research entities.

At Italian level ISCRA is the major program allocating HPC resource facilities for academics of all disciplines: from Biology, Bioinformatics and Biochemistry to Astronomy and Astrophysics, Earth Science, Mathematics and Computer Science, Engineering, Condensed Matter and Fundamental Physics, Computational and Theoretical Chemistry, Materials, Nanosciences, Fluid Dynamics etc.

Applications to ISCRA are currently of two categories: C (up to 1 Million CPU hours), B (between 1M and 10Million). Larger projects initially submitted to ISCRA as class A have currently to be submitted to PRACE. The size of the grant has significantly increased from the initial calls accompanying the growth of researchers needs and the improvement in handling parallel computing resources. Resources are awarded on a competitive basis and all applications are refereed. In an effort to streamline the process, type C applications are only technically reviewed by Cineca, while each B type proposal is also evaluated scientifically by two experts. All applications with their grades are then examined and prioritized by the ISCRA Scientific Committee formed by around twenty experts representing all major scientific areas.

The selection is based on scientific merit, keeping into account originality, innovation potential, scientific excellence, qualification and competence of the proponents, international and national relevance and congruity between requested resources and the objectives of proposal. No preliminary apportioning between disciplines or provenience is made. In summary a rigorous peer review system is implemented.

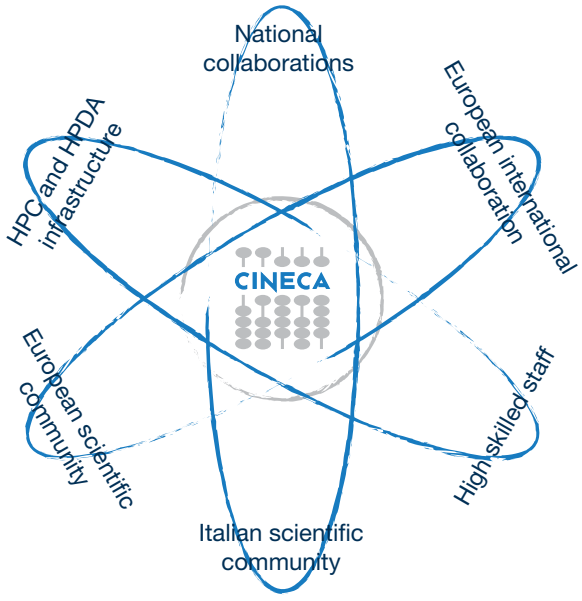
Applications come from the traditional areas of computational condensed matter physics, chemistry, biology as shown elsewhere in the report.

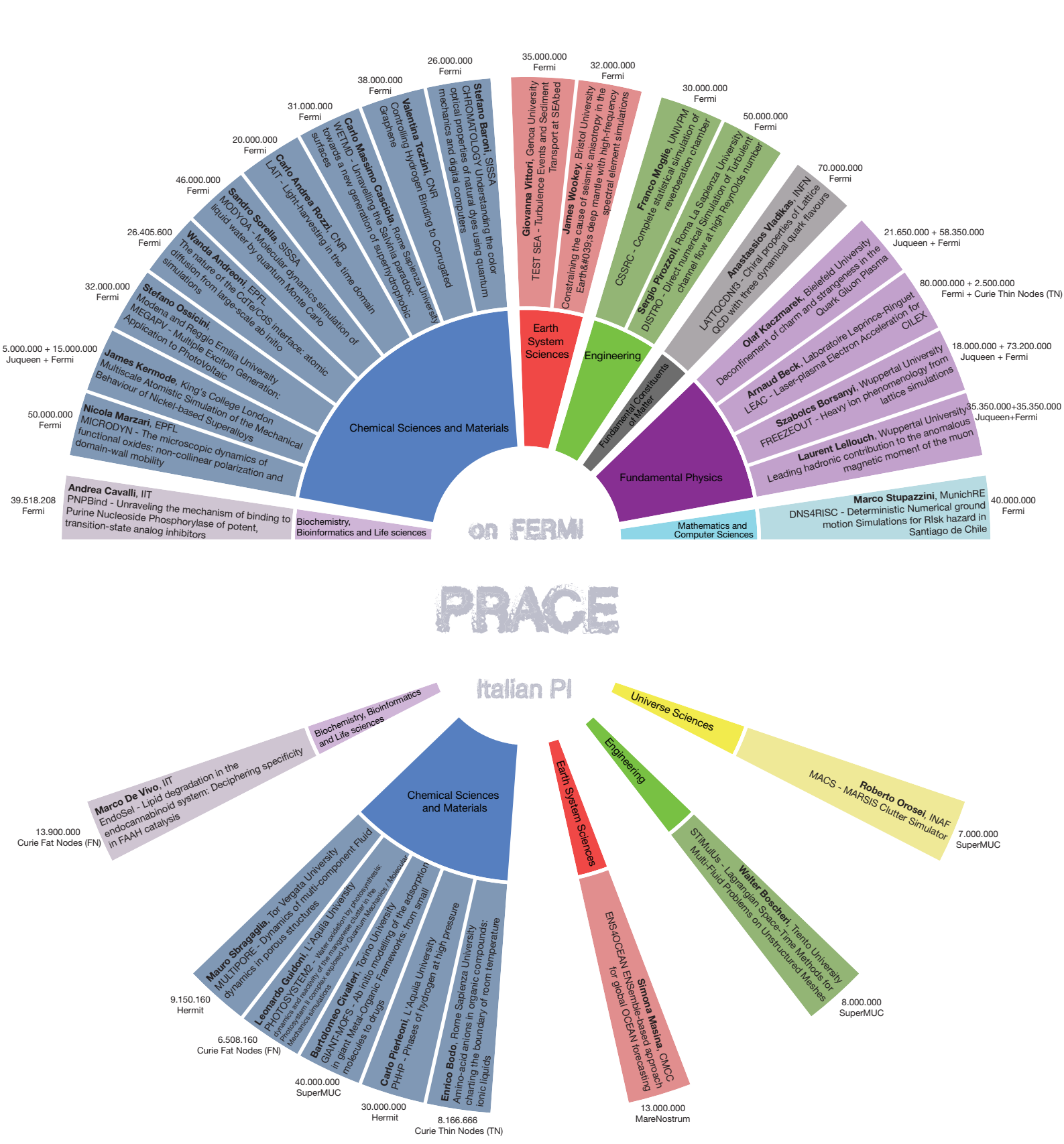
It is worth noticing that a very significant support to researchers requesting it, is offered by the in-house SCAI experts in all the phases of the research work, in the optimization of the codes, in the testing of their effectiveness and scalability, in the drafting of the proposal, as well as, of course, in the implementation of the research on the systems, for ensuring the best exploitation of the machines. This is in accord with one of the missions of SCAI: that of enabling researchers to attack the scientific challenges of their domain, focusing only on science while benefiting, for all HPC and now for HPCD matters, from the extensive experience and specialized skills of the SCAI staff.

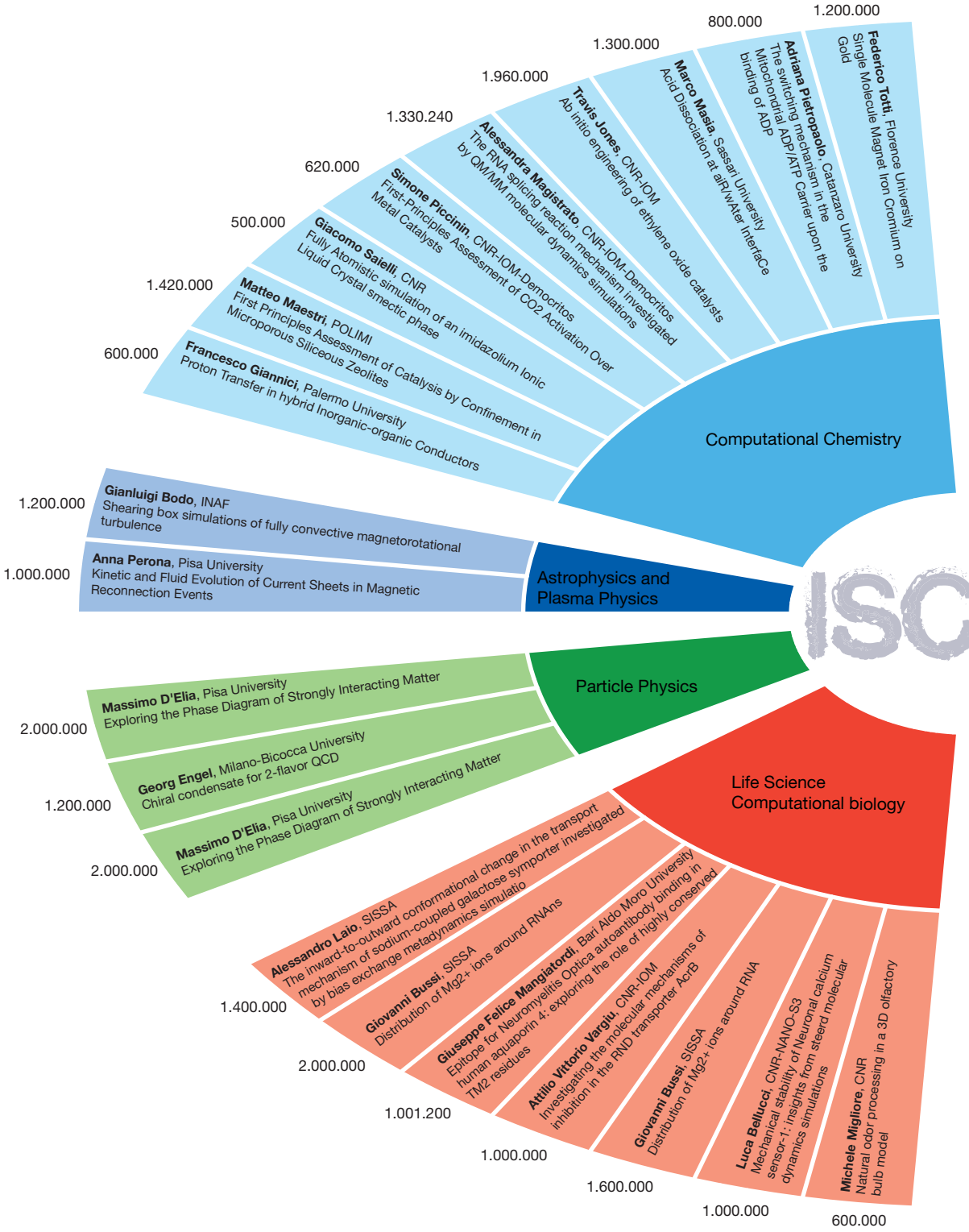
In the following pages we are glad to offer you a selection (made on the basis of the availability of the data at the time of this publication) of the reports that we require to each Principal Investigator, in order to share and disseminate the results of the project. The reports (some included in full, others only as abstracts) refer to users selected via ISCRA and LISA at the national level, and through PRACE at the European level.

Regarding the PRACE projects, the charts offer an overview of all the Italian PIs who obtained an award on any of the PRACE Tier-0 systems, as well as a picture of all the PIs, Italian and worldwide, who have received an award through PRACE on FERMI at Cineca.

Claudio Zannoni
Chairman Scientific Panel




Chemical Sciences and Materials
Earth System Sciences
Engineering
Fundamental Constituents of Matter
Fundamental Physics
Mathematics and Computer Sciences
Biochemistry, Bioinformatics and Life sciences
Andrea Cavalli, IIT
PNPBind - Unraveling the mechanism of binding to Purine Nucleoside Phosphorylase of potent, transition-state analog inhibitors
39.518.208 Fermi
Nicola Marzari, EPFL
MICRODYN - The microscopic dynamics of functional oxides: non-collinear polarization and domain-wall mobility
50.000.000 Fermi
James Kermode, King's College London
Multiscale Atomistic Simulation of the Mechanical Behaviour of Nickel-based Superalloys
5.000.000 + 15.000.000 Juqueen + Fermi
Stefano Ossicini, Modena and Reggio Emilia University
MEGAPV - Multiple Exciton Generation: Application to PhotoVoltaic
32.000.000 Fermi
Wanda Andreoni, EPFL
The nature of the CdTe/CdS interface: atomic diffusion from large-scale ab initio simulations
26.405.600 Fermi
Sandro Sorella, SISSA
MODYQA - Molecular dynamics simulation of liquid water by quantum Monte Carlo
46.000.000 Fermi
Carlo Andrea Rozzi, CNR
LAIT - Light-harvesting in the time domain
20.000.000 Fermi
Carlo Massimo Cavaliola, Rome Sapienza University
WETMD - Unravelling the Salvinia paradox: towards a new generation of superhydrophobic surfaces
31.000.000 Fermi
Valentina Tozzini, CNR
Controlling Hydrogen Binding to Corrugated Graphene
38.000.000 Fermi
Stefano Baroni, SISSA
CHROMATOLOGY Understanding the color optical properties of natural dyes using quantum mechanics and digital computers
26.000.000 Fermi
Giovanna Vittori, Genoa University
TEST SEA - Turbulence Events and Sediment Transport at SEAbed
35.000.000 Fermi
James Wookey, Bristol University
Constraining the cause of seismic anisotropy in the Earth's deep mantle with high-frequency spectral element simulations
32.000.000 Fermi
Franco Magnie, UNIVPM
CSSRC - Complete statistical simulation of reverberation chamber
30.000.000 Fermi
Sergio Pirozzoli, Roma La Sapienza University
DISTRO - Direct numerical Simulation of Turbulent channel flow at high ReynOlds number
50.000.000 Fermi
Anastassios Vladikas, INFN
LATTQCDN3 - Chiral properties of Lattice QCD with three dynamical quark flavours
70.000.000 Fermi
Olaf Kaczmarek, Bielefeld University
Deconfinement of charm and strangeness in the Quark Gluon Plasma
21.650.000 + 58.350.000 Juqueen + Fermi
Arnaud Beck, Laboratoire Leprince-Ringuet
LEAC - Laser-plasma Electron Acceleration for CILEX
80.000.000 + 2.500.000 Fermi + Curie Thin Nodes (TN)
Szabolcs Borsanyi, Wuppertal University
FREEZEOUT - Heavy ion phenomenology from lattice simulations
18.000.000 + 73.200.000 Juqueen + Fermi
Laurent Lellouch, Wuppertal University
Leading hadronic contribution to the anomalous magnetic moment of the muon
35.350.000+35.350.000 Juqueen+Fermi
Marco Stupazzini, MunichRE
DNS4RISC - Deterministic Numerical ground motion Simulations for RIsk hazard in Santiago de Chile
40.000.000 Fermi
on FERMI
PRACE
Italian PI
Chemical Sciences and Materials
Earth System Sciences
Engineering
Universe Sciences
Biochemistry, Bioinformatics and Life sciences
Marco De Vivo, IIT
EndoSel - Lipid degradation in the endocannabinoid system: Deciphering specificity in FAAH catalysis
13.900.000 Curie Fat Nodes (FN)
Mauro Sbragaglia, Tor Vergata University
MULTIPORE - Dynamics of multi-component Fluid dynamics in porous structures
9.150.160 Hermit
Leonardo Guidoni, L'Aquila University
PHOTOSYSTEM2 - Water oxidation by photosynthesis: dynamics and reactivity of the manganese cluster in the Photosystem II complex employed by Quantum Mechanics / Molecular Mechanics simulations
6.508.160 Curie Fat Nodes (FN)
Bartolomeo Civalleri, Torino University
GIANT-MOFS - Ab initio modelling of the adsorption in giant Metal-Organic Frameworks: from small molecules to drugs
40.000.000 SuperMUC
Carlo Pierleoni, L'Aquila University
PHHP - Phases of hydrogen at high pressure
30.000.000 Hermit
Enrico Bodo, Rome Sapienza University
Amino-acid anions in organic compounds: charting the boundary of room temperature ionic liquids
8.166.666 Curie Thin Nodes (TN)
Simona Masina, CMCC
ENS4OCEAN ENSemble-based approach for global OCEAN forecasting
13.000.000 MareNostrum
Walter Boscheri, Trento University
STiMulUs - Lagrangian Space-Time Methods for Multi-Fluid Problems on Unstructured Meshes
8.000.000 SuperMUC
Roberto Orosei, INAF
MACS - MARSIS Clutter Simulator
7.000.000 SuperMUC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Single Molecule Magnet Iron Cromium on Gold
Adriana Pietropaolo, Catanzaro University
The switching mechanism in the Mitochondrial ADP/ATP Carrier upon the binding of ADP
Marco Masia, Sassari University
Acid Dissociation at aiRwAter InterfaCe
Travis Jones, CNR-IOM
Ab initio engineering of ethylene oxide catalysts
Alessandra Magistrato, CNR-IOM-Democritos
The RNA splicing reaction mechanism investigated by QM/MM molecular dynamics simulations
Simone Piccinin, CNR-IOM-Democritos
First-Principles Assessment of CO2 Activation Over Metal Catalysts
Giacomo Saielli, CNR
Fully Atomistic simulation of an imidazolium Ionic Liquid Crystal smectic phase
Matteo Maestri, POLIMI
First Principles Assessment of Catalysis by Confinement in Microporous Siliceous Zeolites
Francesco Giannici, Palermo University
Proton Transfer in hybrid Inorganic-organic Conductors
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Gianluigi Bodo, INAF
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Kinetic and Fluid Evolution of Current Sheets in Magnetic Reconnection Events
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Massimo D'Elia, Pisa University
Exploring the Phase Diagram of Strongly Interacting Matter
Georg Engel, Milano-Bicocca University
Chiral condensate for 2-flavor QCD
Massimo D'Elia, Pisa University
Exploring the Phase Diagram of Strongly Interacting Matter
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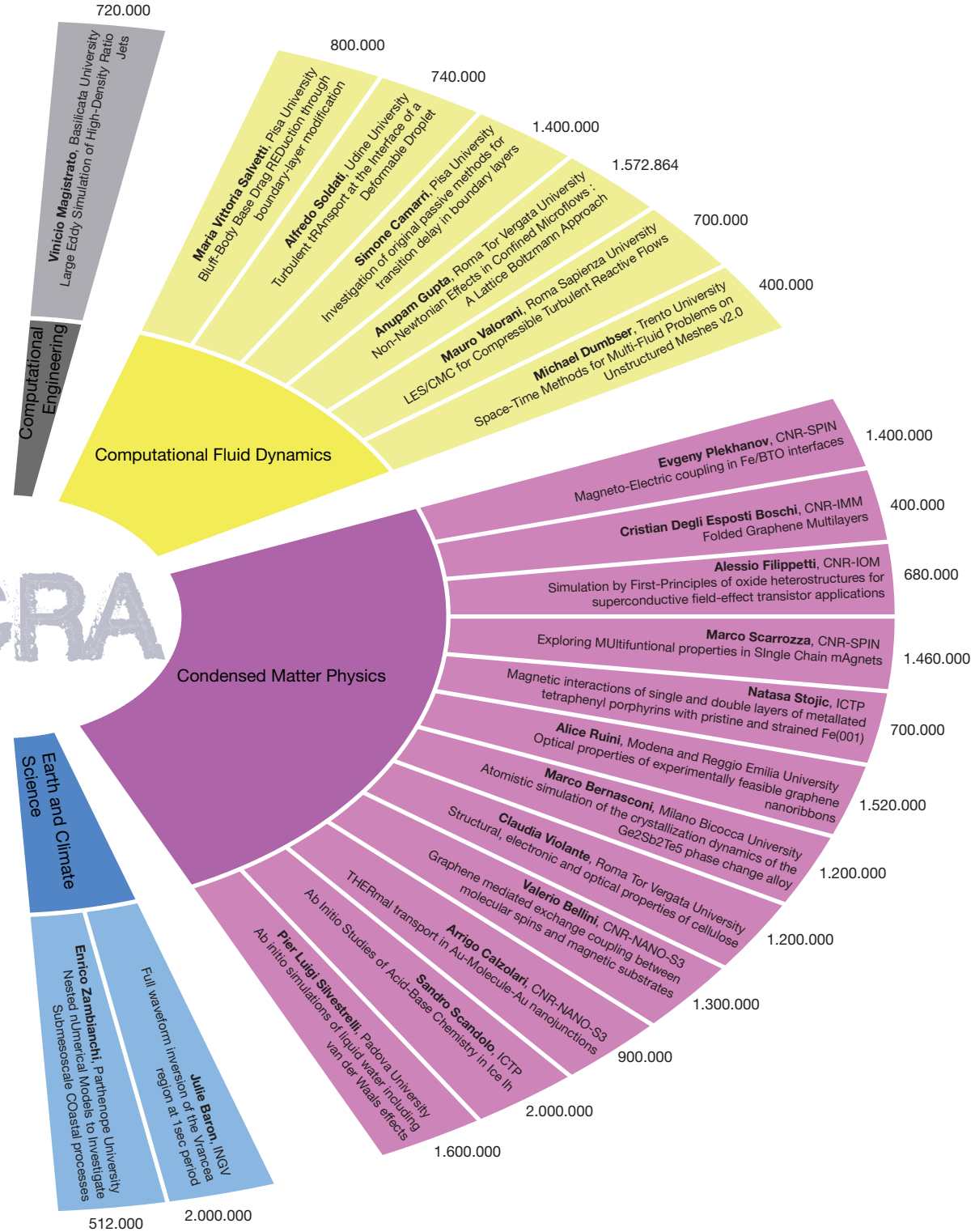
Alessandro Laio, SISSA
The inward-to-outward conformational change in the transport mechanism of sodium-coupled galactose symporter investigated by bias exchange metadynamics simulatio
Giovanni Bussi, SISSA
Distribution of Mg2+ ions around RNAns
Giuseppe Felice Mangiatordi, Bari Aldo Moro University
Epitope for Neuromyelitis Optica autoantibody binding in human aquaporin 4: exploring the role of highly conserved TM2 residues
Attilio Vittorio Vargiu, CNR-IOM
Investigating the molecular mechanisms of inhibition in the RND transporter AcrB
Giovanni Bussi, SISSA
Distribution of Mg2+ ions around RNA
Luca Bellucci, CNR-NANO-S3
Mechanical stability of Neuronal calcium sensor-1: insights from steerd molecular dynamics simulations
Michele Migliore, CNR
Natural odor processing in a 3D olfactory bulb model
Life Science
Computational biology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Alfredo Soldati, Udine University
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Simone Camarri, Pisa University
Investigation of original passive methods for transition delay in boundary layers
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Anupam Gupta, Roma Tor Vergata University
Non-Newtonian Effects in Confined Microflows : A Lattice Boltzmann Approach
700.000
Mauro Valorani, Roma Sapienza University
LES/CMC for Compressible Turbulent Reactive Flows
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Michael Dumbser, Trento University
Space-Time Methods for Multi-Fluid Problems on Unstructured Meshes v2.0
Computational Engineering
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Evgeny Plekhanov, CNR-SPIN
Magneto-Electric coupling in Fe/BTO interfaces
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Cristian Degli Esposti Boschi, CNR-IMM
Folded Graphene Multilayers
680.000
Alessio Filippetti, CNR-IOM
Simulation by First-Principles of oxide heterostructures for superconductive field-effect transistor applications
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Marco Scarrozza, CNR-SPIN
Exploring MUltifuntional properties in SIngle Chain mAgnets
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Natasa Stojic, ICTP
Magnetic interactions of single and double layers of metallated tetraphenyl porphyrins with pristine and strained Fe(001)
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Alice Ruini, Modena and Reggio Emilia University
Optical properties of experimentally feasible graphene nanoribbons
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Marco Bernasconi, Milano Bicocca University
Atomistic simulation of the crystallization dynamics of the Ge2Sb2Te5 phase change alloy
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Claudia Violante, Roma Tor Vergata University
Structural, electronic and optical properties of cellulose
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Valerio Bellini, CNR-NANO-S3
Graphene mediated exchange coupling between molecular spins and magnetic substrates
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Arrigo Calzolari, CNR-NANO-S3
THERmal transport in Au-Molecule-Au nanojunctions
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Sandro Scandolo, ICTP
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Pier Luigi Silvestrelli, Padova University
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Earth and Climate Science
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Enrico Zambianchi, Parthenope University
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Julie Baron, INGV
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Understanding the color of flowers using quantum mechanics and digital computers

Color perception is a pervasive feature of human cognition and has an immense impact in the visual arts, in the natural sciences, and in such diverse economic activities as agriculture or textile, painting, makeup, and food industries. Many traditional colorants are toxic (e.g. they may contain heavy metals), hence their use in food and pharmaceutical industries or in cosmetics would be dangerous. In this regard, natural dyes (such as, chlorophylls, anthocyanins, and carotenoids) may be a valid alternative. Anthocyanins, in particular, are a class of natural dyes responsible for the characteristic coloration of many fruits, vegetables, and flowers, as well as of the red and purple shades in the leaves of plants. The multitude of colors that these dyes express results from a complex range of factors, including the substituents of the aromatic rings, the acidity of the solution, its temperature, as well as the presence of metal cations and/or co-pigmentations. The prospect of replacing many toxic or potentially dangerous artificial dyes with natural substitutes relies on our ability to understand and engineer the many factors on which the color expressed by a given dye depend. Unfortunately, very little is known on the molecular basis of the color optical properties of natural dyes, and the complexity of the environment in which these systems perform their optical function make their simulation extremely difficult. Only very recently, has it been possible to combine state-of-the-art quantum simulation techniques such as Car-Parrinello molecular dynamics and the Liouville-Lanczos approach to time-dependent density-functional theory to predict the color optical properties of a few representative anthocyanins in solution. In spite of these substantial methodological advances, the numerical complexity of the simulation is such that it could not tackled without the availability of massively parallel computers as the BG/Q Fermi machine at Cineca, and the existence of the PRACE access program to this kind of computer resources. In Figure we display a few representative results obtained in the PRACE project CHROMATOLOGY in which we have been able to predict, for the first time entirely from first principles, the color optical properties of a few anthocyanins in solution. The figure (panel a) below displays a snapshot of a 10ps-long Car-Parrinello molecular dynamics trajectory, during which absorption spectra were collected on the fly every 0.5 ps. The simulation cell includes the target molecule (namely cyanin) and a layer including ~170 water molecules (i.e. 565 atoms and 1538 electrons). The correct treatment of the electronic structure requires also the inclusion of hybrid XC-functionals (B3LYP) in the simulation of the TDDFT spectra. The resulting-time averaged spectra can be directly compared with the experimental one, as shown in panel b. Once the spectra are collected, the corresponding colors can be easily obtained. Panel c reports the final comparison between theoretical and experimental colors of three different dyes (cyanin, pelargonin and delphinin), which are representative example of anthocyanins with a variable number of oxygens in the chromophore. The agreement between simulated and experimental colors is evidentely excellent.

On the basis of the impressive results for mono-glucoside anthocyanins, we applied the same procedure to a so-called copigmented anthocyanin [RedC: cyanidin-3-(sinapoyl)diglucoside-5-glucoside] in water solution, which plays a relevant role in food industry, as natural colorant. This second set of calculations (~1300 atoms, ~3600 electrons, ~5 milion plane waves) realizes the computational upper limit for this kind ab-initio simulations. A snapshot of the corresponding CPMD trajectory along with the absorption spectrum and the simulated color are shown in panels d and e, respectively.

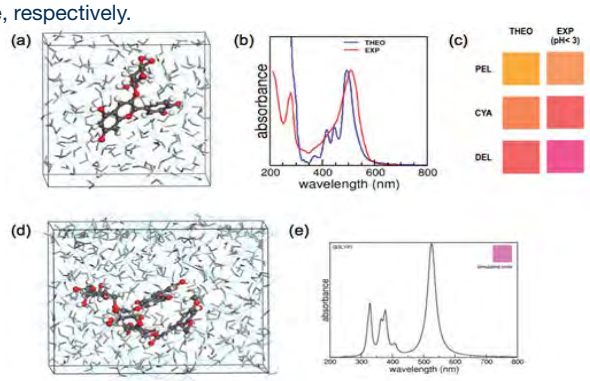


Figure: (a) Atomic structure of solvated cyanin dye, from a single snapshot of CPMD; (b) comparison between theoretical and experimental spectra of solvated cyanin; (c) Color palette for selected anthocyanins: pelargonin (PEL), cyanin (CYA) and delphin (DEL). (d) Atomic structure of solvated co-pigmented RedC dye, from a single snapshot of CPMD; (e) absorption spectrum and simulated color corresponding to snapshot of panel (d).

This project has substantially benefitted not only from the allocation of substantial computer resources from the PRACE initiative, but even more from a very active and long-lasting collaboration with the Cineca technical staff that has allowed to port the Quantum ESPRESSO suite of computer codes to the BG/Q computer, to substantially enhance its performance, and to fine-tune all the system parameters necessary to optimally exploit the capabilities of the BG/Q architecture.

Stefano Baroni
SISSA

Stochastic first principle approach for the simulation of liquid water

There is no doubt about the importance of liquid water for climate and life on Earth. However for the theoretical and computational point of view it remains a challenging material as, after several years from the first ab-initio Car-Parrinello molecular dynamics simulation (1985), no consensus has been reached on what are the basic interactions determining his properties in the solid and especially in the liquid phase at ambient conditions.

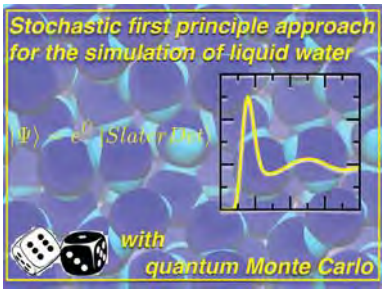
Nowadays, also thanks to the PRACE infrastructure provided by Cineca, we are living in a revolutionary time for high-level quantum Monte Carlo computations. New massively parallel computers with several thousands (32768 in the work) cores can now provide a tremendous boost to the field, but only to those theoretical methods that can profit by this technology. At variance with post-Hartree-Fock methods, computational techniques based on stochastic approaches, such as quantum Monte Carlo, are recently demonstrating to fully exploit the potential offered by these emerging technologies. At the same time, these high-level techniques are able to provide details of the electronic structure of molecules and solids that cannot be tackled by traditional approaches.

In this context, Quantum Monte Carlo methods can offer a high-level fully-correlated description of the electronic structure of hundreds of atoms thanks to a better asymptotic computational cost for large systems with respect to traditional post-Hartree-Fock approaches. So far, quantum Monte Carlo techniques were mainly limited to single structure calculations and only very recently extended to geometry optimizations. In recent years, we have developed an efficient ab-initio molecular dynamics scheme, which allowed to extend these high-level Variational Monte Carlo techniques to the range of finite temperature simulations.

In the present work supported by PRACE we report for the first time an ab-initio molecular dynamics simulation of a fundamental and complex molecular liquid, such as water, based on a highly accurate wave-function-based method. On the ground of the Variational Monte Carlo ab-initio molecular dynamic technique, already applied in a recent paper on high-pressure hydrogen [Nat. Comm 5, 3847 (2014)] (a work supported by the previous PRACE call), we are here able to simulate the room temperature dynamics of liquid water for enough time to measure structural data such as radial distribution functions.

The obtained results are in remarkable agreement with recent neutron scattering experiments, determining the position of the first peak in the oxygen-oxygen radial distribution function with high degree of accuracy $R_{\rm max} \sim 2.80$~\AA, a value that is ~ 0.1~\AA~ off from several previous ab-initio claims. The accordance between our data and these new experiments gives back to ab-initio molecular dynamics the predictive power which has been sometimes weakened by the use of approximate functionals in DFT-based simulations.

In addition to the valuable insights on the properties of liquid water, the present work is a sharp and solid demonstration of how the molecular dynamics based on high-level correlated wave functions is becoming a reality, opening new perspectives in the field of ab-initio simulation of liquids, solids and correlated materials.



Sandro Sorella
SISSA

Massive simulation and complete statistical analysis of reverberation chambers

The numerical simulations of mode-stirred reverberation chamber (RC) were performed using an in-house parallel finite-difference time-domain (FDTD) code. The code is divided into three modules that are managed by a unique, single-step job. Modules are: the electromagnetic solver based on the FDTD method; a fast Fourier transform (FFT) module (based on FFTW library) to obtain the frequency domain behavior; a statistical module to obtain the RC properties. A unique run produces statistical results for all the investigated stirrer angles, without the burden of saving intermediate data. The code implements a hybrid parallelization. In the case of FDTD and FFT modules, MPI protocol has been used to parallelize the RC structure with the stirrer angle, while OpenMP protocol have been used to parallelize the inner volume of the cavity or the single FFT routine. After a data arrangement, the statistical module uses MPI protocol to divide the computation of the whole frequency range in subranges, and OpenMP protocol operates an inner parallelization of the code cycles. Those parameterizations offer the proper platform for realizing the parallel computation. Specifically, such a computation is known to be “embarrassingly parallel” with respect to the stirrer angle or the position of other not fixed objects inside the RC.

We have performed a different number of independent numerical (MPI) simulations, whence the cavity ensemble has been generated rotating the stirrers or placing the objects in some positions inside the RC. When a sole stirrer is employed, its investigated angles are sequential. Conversely, when more than one stirrer are rotating or a tripod or a field probe is moved in a grid the simulations cannot be order in any sequence. This implies different statistic analysis.

The RC wall losses are implemented numerically through an equivalent (volumetric) air-conductivity in the reverberant space. The value of this equivalent conductivity adopted for each set of simulations is selected in the ranges from $\sigma = 2.5\ 10^{-6}$ S/m to $\sigma = 80\ 10^{-6}$ S/m. This implementation allows us to obtain best performance on the Blue Gene/Q architecture maintain the same statistical behavior and a close field distribution.

The time-domain excitation is chosen in such a way as to yield information over a wide enough frequency band. We achieve this aim by employing a Gaussian type distribution centered at the middle of the investigated band. The Gaussian excitation pulse is chosen to have an amplitude spectrum in the range of the operation band. Peak value is at 1.1 GHz while at 0.2 and 2 GHz the value is reduced at 5% of the peak. By this choice, the time pulse is a retarded (to retain causality of excitation) Gaussian pulse which modulates a 1.1 GHz sinusoidal carrier. Time delay is assumed equal to 4 times the standard deviation of the Gaussian pulse. When the time simulation of the FDTD module is completed, the FFT module gives the frequency behavior of the fields in each point of the RC with a frequency resolution of about 50 kHz.

We acknowledge PRACE for awarding us access to resource FERMI based in Italy at Cineca.

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DII - Università Politecnica delle Marche

Gabriele Gradoni
Nottingham University

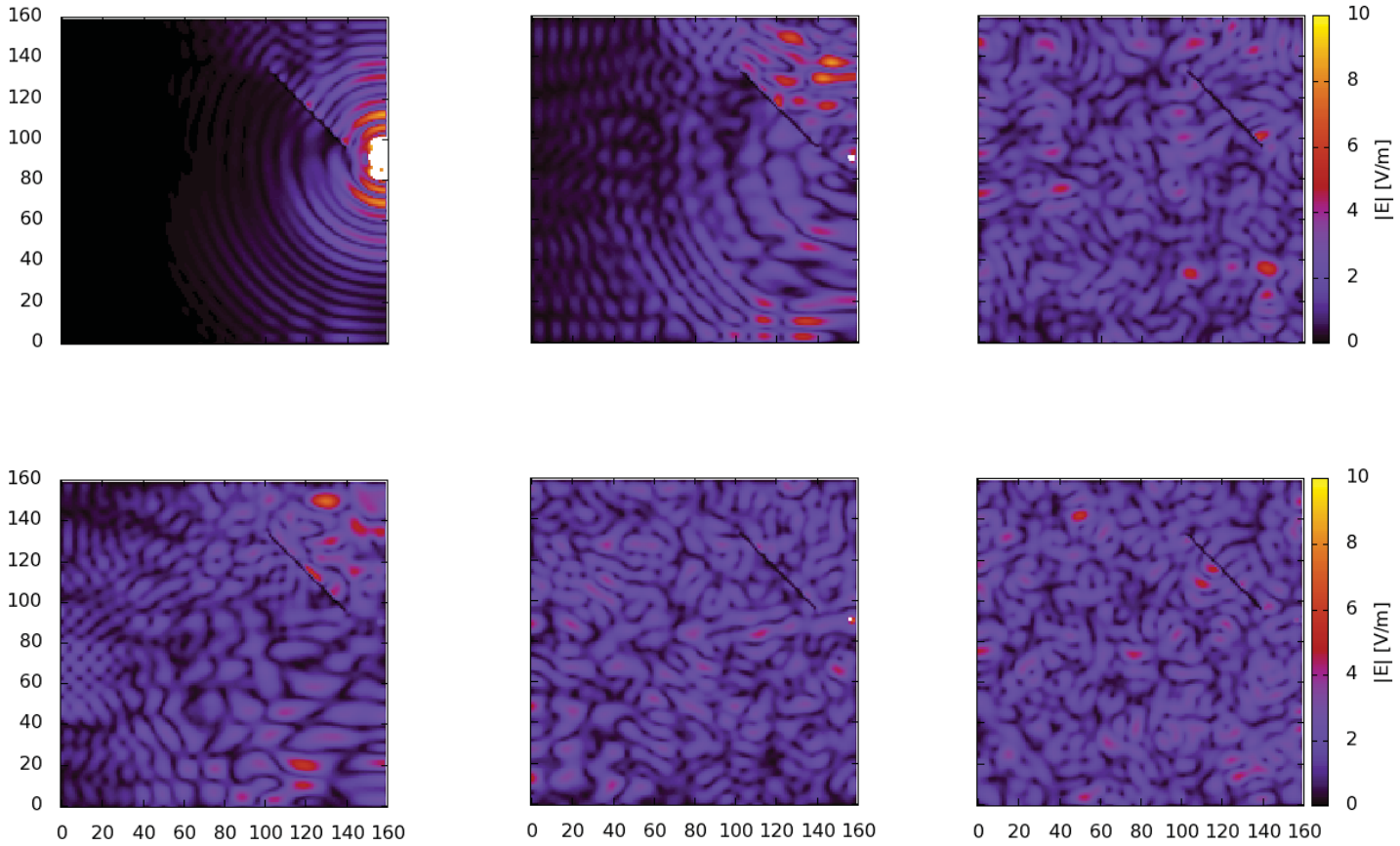


Figure 1: Field pattern captured in six subsequent time instants (5, 10, 15, 20, 25, 30 ns). Axis units are cell number whose size is 15 mm. The build up time of the
chamber is well visible, i.e. the time required to switch the pattern between a deterministic to a chaotic behavior.

Figure 2: Field pattern in a horizontal section of two reverberation chambers coupled by an aperture. Axis units are cell number whose size is 15 mm.

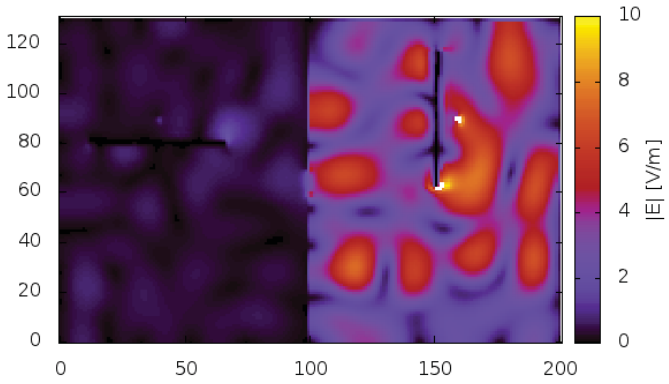
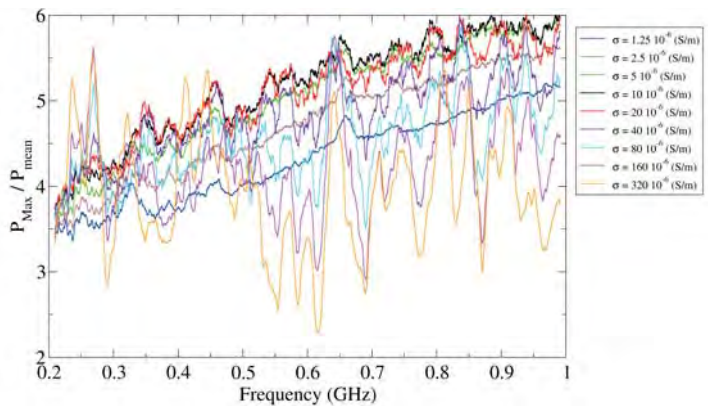


Figure 3: Maximum-to-mean ratio of the received power, as function of the selected air conductivity values. A sliding average over a 100 MHz band is applied.
Results underline an important aspect: the highest value of the ratio is not obtained for the highest value of conductivity, but for an optimal intermediate conductivity level of about 10^{-5} S/m.



Simulations of accretion discs: turbulent transport and dynamo action

The process of accretion, through which matter gradually falls on a central object, is crucial for many astrophysical phenomena. Accretion typically occurs in the form of a disc and we can find accretion discs both in the nuclei of galaxies, around supermassive black holes, and around stars at the beginning and at the end of their life. As accretion proceeds, the matter falling on the central body releases its gravitational energy, that is transformed into heat and into the observed radiation. Accretion discs can power some of the most energetic phenomena in the universe and understanding how they work is very important for the comprehension of different astrophysical problems like how stars are formed or what happens in the central cores of galaxies.

In order to have accretion, however, angular momentum has to be extracted from the matter in the disc, otherwise it would continue to orbit forever around the central object. For this reason, understanding the process of angular momentum extraction is fundamental for determining the mass accretion rate and the disc luminosity. Friction between adjacent rings of the disc, moving at different angular speed, can provide a way to extract angular momentum, but this process is much too slow and the resulting luminosities are well below those we observe. Friction must then be enhanced by turbulent motions and, in order to develop turbulence, the disc must be magnetized, in fact non magnetized discs are known to be stable. On the other hand, turbulence has to regenerate the magnetic field it needs to develop, otherwise it dies and accretion stops, unless an external magnetic field is provided. The analysis of these complex processes can be done only through three-dimensional magnetohydrodynamic simulations that can be only performed on supercomputers of the class of PRACE systems.

In our project we followed the rotation of a small portion of the disc at very high resolution, in order to capture the turbulence at very small scale, and we also studied the dynamics of the global disc. The simulations were performed with the PLUTO code, developed by our group, with computational boxes of up to 30,000,000 grid cells, on more than 32,000 cores of FERMI Blue Gene/Q at Cineca.

First, looking at a small patch of the disc, we studied how the heat generated inside the disc is carried out to the surface to be radiated and we discovered that this is accomplished by convection, very much like in a pot of boiling water. Furthermore, the presence of convection helps turbulent motions to regenerate magnetic field by a dynamo process and thus enhances the overall efficiency of the accretion process. The global disc simulations show a similar convective behavior and how it changes with radial distance from the central body, furthermore it shows the formation of a spiral structure of the magnetic field. The scientific results that we have obtained, have been collected in a series of paper published in International Journals. This project has been successful in adding a new tile in the comprehension of how the interplay between turbulence, magnetic field generation, energy transport by convection makes accretion work in the most diverse astrophysical environments.

Gianluigi Bodo, Paola Rossi
INAF Torino Astrophysical Observatory

Andrea Mignone
Torino University

Figure 1: The figure shows the relation between the global disc simulations (on the right) and the local patch simulation (on the left). The color scale represents the temperature distribution, lighter regions are hotter, while darker regions are cooler. The top surface shows the pattern of convective cells, lighter regions are where the hotter material is flowing upwards, while the darker regions are where the cooler material is flowing down.

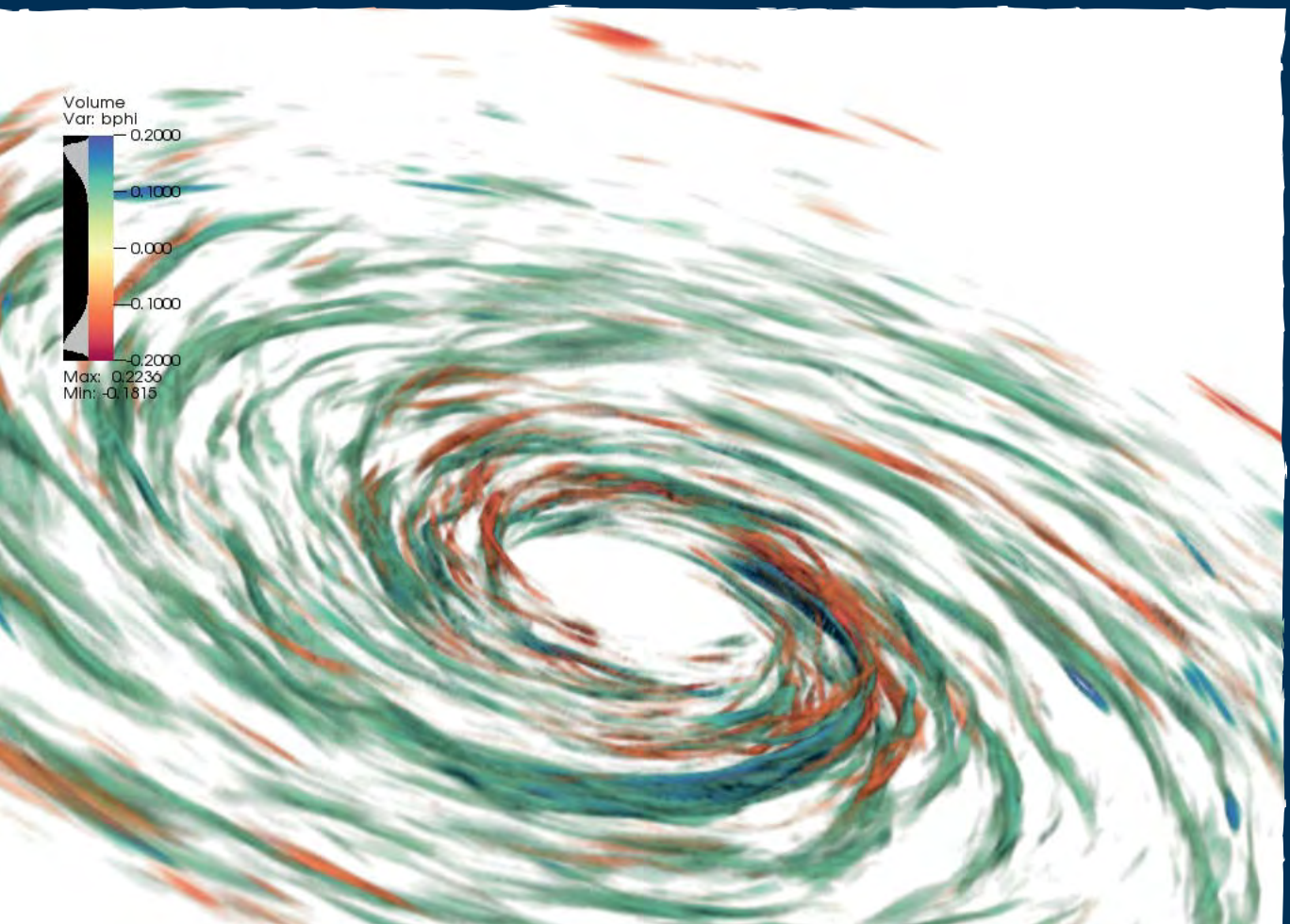


Figure 2: Structure of the magnetic field in the global disc.

3DMagRoI: High-resolution 3D study of MRI in relativistic rotating stars

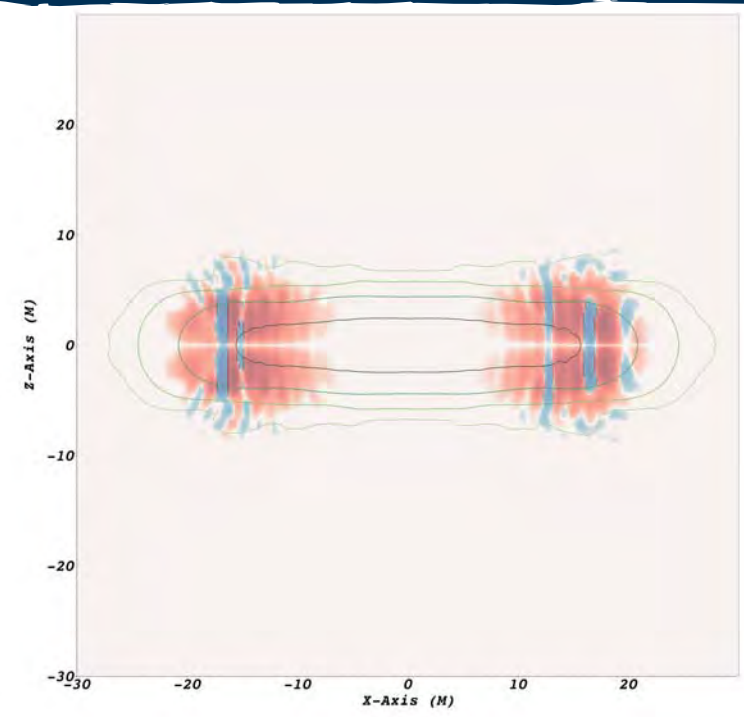
Many of the most fascinating high-energy phenomena present in our universe, such as Gamma-Ray Burst (GRBs), are associated with strong magnetic fields and fast rotating compact objects. In particular, the recently developed millisecond-magnetar model has suggested that such violent events might be the signature of a rapidly rotating and highly magnetized neutron star (NS). Although the origin of these strong and ordered magnetic fields remains poorly understood and this project aimed to try to understand how extremely strong magnetic fields (of the order of 10^{16} Gauss) may arise as a result of hydro-magnetic instabilities, like the Magneto-Rotational-Instabilities (MRI), in an environment characterized by turbulence, instabilities and convection, still simple models of GRBs jet launching make strong predictions on the strength and geometry of the field in the engine.

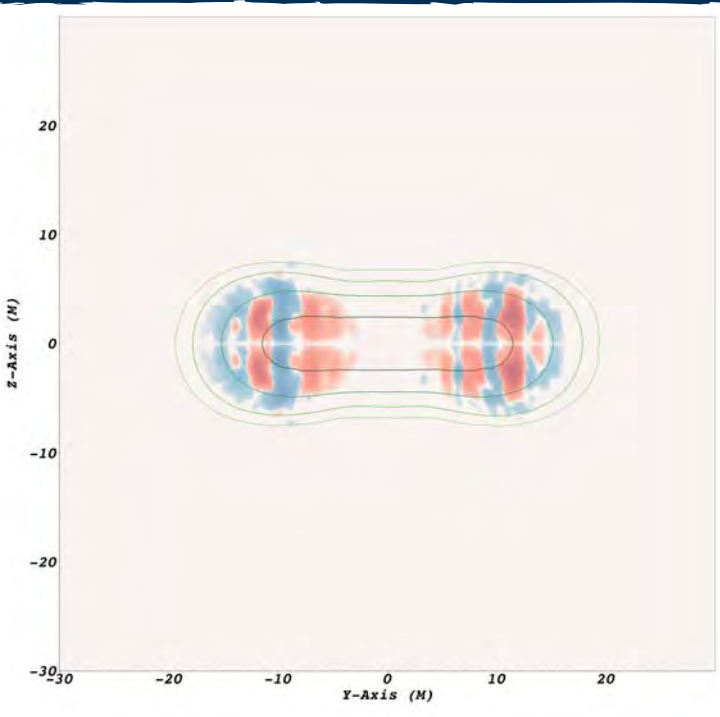
This project involved high-resolution 3D simulations in full General Relativity to study the effects that magnetic fields may have on the dynamics of magnetized differentially rotating neutron stars. In particular, in the case of an initial weak field, our main goal was to follow the onset and growth of the magneto-rotational instability (MRI) that is supposed to redistribute the angular momentum of the star and to amplify the magnetic field. Among others we evolved a series of stellar models which are bar-mode unstable, i.e. unstable for m=2 matter deformations, and characterized by different values of the initial magnetic fields strength in the range between 1011 Gauss and 1014 Gauss and a fixed resolution of dx=0.378 km. We also performed five simulations of a bar-deformation unstable stellar model (namely U13-1.0e14), which has a seed poloidal magnetic field of 1014 Gauss at different resolutions between dx=0.295 km and dx=1.180 km. In all these evolved models, the growth of the toroidal magnetic field component is linear in time initially, as a result of the winding of the field lines due to the “freezing” condition within the ideal-MHD approximation which forces the magnetic field to follow the fluid in its motion. The toroidal component then, becomes rapidly larger than the initial poloidal one and an amplification of the toroidal electromagnetic energy of more than two orders of magnitude takes place. Afterwards, during the matter-unstable phase, i.e. once the star has lost the initial axisymmetry, the toroidal component of the magnetic energy shows a sudden increase, namely an exponential growth, reaching a higher value of about 50%.

Our investigation showed (see Figure 1) that MRI instabilities do activate during matter unstable phases but in general seems not able to last as much as it is needed in order to produce magnetic fields amplification of the order required to justify GRBs jet launching from the dynamics inside the star. Moreover, they seems not to survive against other instabilities and still a large number of questions are still open: whether a large dipolar component can be generated or higher multipoles are found to dominate; how much magnetic energy can be stored inside the NS and whether this energy can be released at later times to power the afterglow activity; whether a strong magnetic field introduces deformations in gravitational wave signals; whether these waves can take away a large fraction of the rotational energy of the NS, quenching the engine.

Roberto De Pietri
Parma University and INFN Parma

Snapshot of the amplitude of the radial component of magnetic fields at time t=13.5 ms of the evolution of the stellar model U13-1.0e14. Please note, in the two sections on the xz-plane and yz-plane, the typical “wave” structure expected in the presence of MRIs.





PRACE

Sailing Before the Light: LSAIL Large Scale Simulations of Ion Acceleration by Laser

The idea of using large, thin mirrors as “light sails” to navigate the solar system by exploiting the boost from the radiation pressure of the Sun dates back to 1925 (F. A. Zander). In the early sixties, the invention of the laser suggested to exploit an Earth-based laser system for boosting a ship up to the nearest star. Such visionary idea was stimulated by the high efficiency of light sails as their velocity approaches the speed of light. Presently the same concept, scaled down to sub-picosecond times and sub-mm distances and using ultra-powerful lasers is being investigated as a novel laser accelerator of high energy ions.

One aim of the LSAIL project was to simulate light sail acceleration in conditions as realistic as possible, for parameters typical of next generation high power laser systems such as those planned in the Extreme Light Infrastructure (ELI) EU project. Performing three-dimensional simulations is thus essential, also because theory shows that low-dimensional models may actually underestimate the final ion energy for given laser and target parameters due the importance of the target expansion dynamics.

Particle-In-Cell (PIC) simulations were performed on up to 16384 cores on FERMI at Cineca. For the cases shown, the grid size was 4096 X 1792 X 1792 and 128 particles per grid cell were used yielding a total number of about 2 X 10^{10}. These runs allowed to demonstrate for the first time in 3D simulations a high energy gain regime which may allow to produce multi-GeV ions with ELI-class lasers. They also showed that the ion density becomes strongly modulated as a result of a particular type of Rayleigh-Taylor instability (RTI), seeded by plasmonics effects. While the RTI may be an issue for optimizing ion acceleration, the particular structures observed as resulting from the nonlinear RTI evolution provided an original example of self-organization and spontaneous symmetry breaking in a classical system.

The PIC simulations were performed using the codes AlaDyn (originally developed by P. Londrillo, C. Benedetti et al) and PICcante, an open source project (https://github.com/ALaDyn/piccante).

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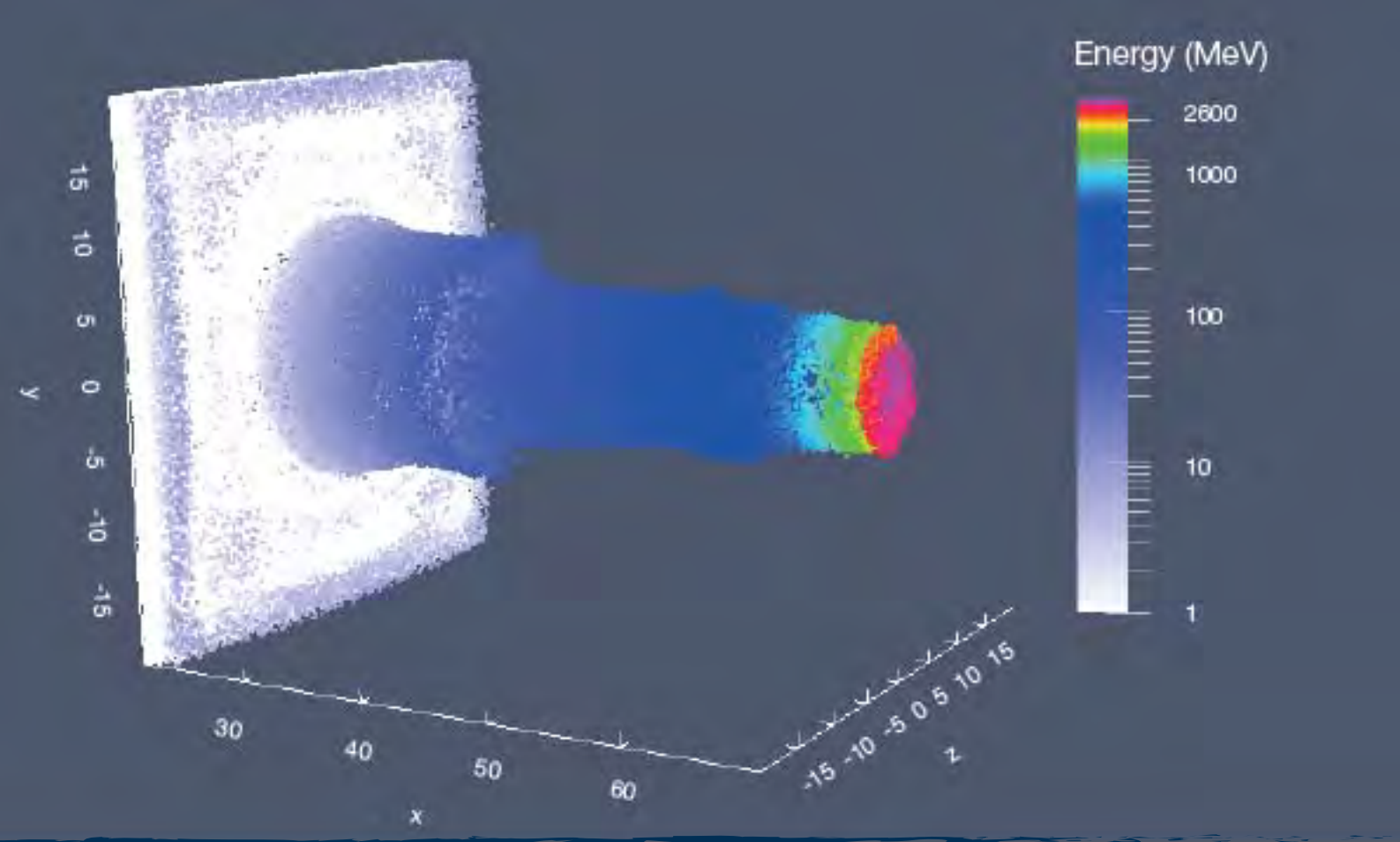
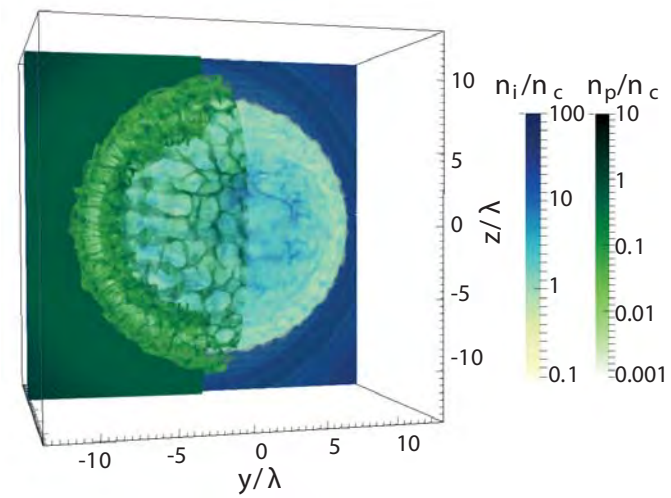


Figure 1: Distribution of protons in 3D space and in energy (colors) from the simulation of the interaction of a 8.5 X 10^{22} W/cm^2, 24 fs laser pulse with a thin solid hydrogen foil.

Figure 2: Density distribution of protons and carbon ions for a two-species target: simulation parameters are the same as Fig.1. The structures are due to the nonlinear development of a Rayleigh-Taylor instability.



Direct numerical simulation of turbulent channel flow at high Reynolds number

A DNS database of turbulent channel flows has been recently built by our group through large-scale, massively parallel simulations, performed at Cineca under the ISCRA and the PRACE initiatives. The main scientific goal is to explore a range of Reynolds numbers (given in terms of Re_τ , the ratio of the channel-half height, h, to the wall viscous scale δ_ν) not achieved so far, thus probing phenomena which should be typical of the asymptotic high-Reynolds-number regime. Specifically, the main overarching questions are as follows: i) does a logarithmic layer appear in the velocity profiles?; ii) what is the effect of large-scale coherent structures sitting off the wall on the near-wall structures? As shown below, the present set of simulations have helped to shed light on these two fundamental issues.

The numerical code solves the incompressible Navier-Stokes equations in a channel by enforcing a constant mass flow rate [Bernardini et al., 2013], and it is based on a staggered finite-difference arrangement of the flow variables, thus guaranteeing that kinetic energy is discretely conserved in the limit of inviscid flow [Pirozzoli et al., 2010]. Details on the flow parameters for the DNS are provided in table 1.

Flow case	Re_τ	N_x	N_y	N_z	$\Delta x/\delta_v$	$\Delta z/\delta_v$
P1	546	1024	256	512	10.0	6.7
P2	999	2048	384	1024	9.2	6.1
P3	2012	4096	768	2048	9.3	6.2
P4	4079	8192	1024	4096	9.4	6.2

Table 1: List of parameters for turbulent channel flows. $Rey_\tau = h/dv$ is the friction Reynolds number, N_i is the number of collocation points in the i-th direction, and the corresponding resolution Δx_i is given in units of δ_v.

The mean velocity profiles for the simulations are shown as a function of the wall distance (y) in Fig. 1(a), and compared with recent experimental data [Schultz and Flack, 2013]. Figure 1 highlights the onset of a layer with nearly logarithmic velocity variation, whose extent visually increases with Re_τ, and excellent agreement with experiments. More refined information on the behavior of the mean velocity profile can be gained from inspection of the log-law diagnostic function $\Xi = y d\bar{u}/dy$, shown in figure 1(b), whose constancy would imply the formation of a logarithmic layer in the mean velocity profile. The figure supports universality of the mean velocity in inner units up to $y \approx 100$ dv, where the diagnostic function attains a minimum, and the presence of a maximum whose position scales in outer units, at $y/h \approx 0.5$. An extended range of linear variation of the diagnostic function is observed in the outer layer in the high-Re data here presented, as could not be observed before, and which is consistent with the refined overlap arguments of Afzal and Yajnik [1973], who proposed that

$$\Xi = 1/k + \alpha y/h + \beta/Re_\tau, \quad (1)$$

where α, β are adjustable constants, and k is the equivalent of the K´arm´an constant. Fitting the DNS data we find $k = 0.41$, $\alpha = 1.15$, $\beta = 180$, which can be regarded as an extended form of the logarithmic log law. The main conclusion is that a genuine logarithmic layer is not achieved at any finite Reynolds number Bernardini et al. [2014], which is in contrast with typical expectations based on low-Re data.

A visual impression of the effect of outer-scaled coherent motions on the near-wall layer can be gained from flow visualizations as Fig. 2, where we show velocity fluctuation contours in wall-parallel planes at $y = 0.3\ h$ (i.e. in the outer layer) and at $y \approx 15\ \delta_v$ (i.e. in the wall proximity). While the former show the presence of large-scale motions with size comparable to the channel height, a two-scale organization emerges near the wall, with high- and low-momentum streaks having size of the order of $100\delta_v$, and superposed on them much larger streaks, which are the clear imprint of the outer-layer eddies of Fig. 2(a). Although this effect was previously noticed in DNS at lower Reynolds number, the scale separation and imprinting effects here are much more evident.

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Flow in turbulent channel at Re_τ = 4000: visualization of temperature field in representative planes. The channel is periodic in the *x* and *z* directions, and y is the wall-normal direction. The color scale ranges from blue (cool fluid) to red (hot fluid). The figure well highlights the presence of large coherent eddies in the core flow, and their imprint onto the near-wall flow, which is characterized by a sea of small-size streaks.

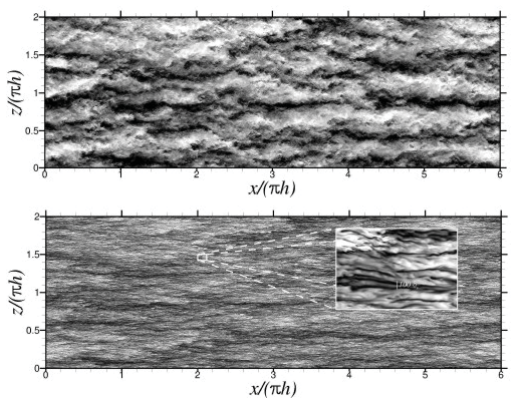
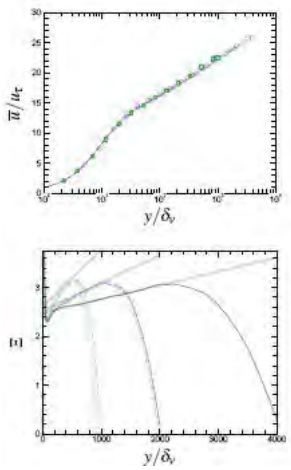


Figure 2: Instantaneous streamwise velocity field in wall-parallel planes at y/h = 0.3 (a) and $y/\delta v$ = 15 (b), for the P4 dataset. Contour levels are shown for $-2.3 \le u'/u_\tau \le 2.3$ (a), and $-1.56 \le u'/u_\beta \le 1.56$ (b), from dark to light shades. The figure inset in (a) shows a zoom of a ($1500\delta_\nu \times 1000\delta_\nu$) box, to highlight viscous length scales.

Figure 1: Mean velocity profile (a) and associated diagnostic function (b). In (a) the symbols indicate experimental data from Schultz and Flack [2013], at Re_τ =1010 (squares), Re_τ =1956 (diamonds), Re_τ =4048 (circles). In (b) the thick grey lines correspond to the generalized logarithmic profiles defined in equation (1), for Re_τ corresponding to the P2-4 DNS; the symbols correspond to the DNS data of Hoyas and Jiménez [2006].



Nano-scale corrugation of graphene: structure, electronic properties and interaction with hydrogen

Since the Nobel Prize for Physics 2010 awarded for the discovery of graphene, this two dimensional material, extremely resistant and very fast electricity conductor (1). However, perhaps the most peculiar property is its flexibility: at the macroscopic level graphene maintains its conduction properties even when bent, which has boosted the field of flexible electronics (2). On the other hand, when corrugation is at the nanometer scale, the curvature radius is proportionally reduced, leading to new phenomena. This is precisely the domain we investigated by means of a computational study based on Density Functional Theory, using FERMI HPC system by means of the PRACE award Pra07_1544.

Naturally nano-scale corrugation is obtained in graphene grown on Silicon Carbide substrate (SiC) by Si evaporation (see Figure (a)). Both the "buffer layer" covalently bound to the substrate and the first monolayer graphene are rippled due to a mismatch of the lattice parameters of SiC and graphene. We first optimized model systems reproducing ripples of the same size and geometry, both with (Figure (a)) and without the substrate (Figure (b)), in the latter case by lateral compression and appropriate supercell size and geometry. The second model system is relatively computationally cheap, allowing a systematic study in a large range of curvature levels, by changing the compression. We found that graphene reactivity, for instance towards hydrogen chemisorption, is enhanced on convex sites (3,4), proportionally to the local curvature. This is because convex sites have a structure nearer to "pyramidal" one assumed when hydrogen is attached. This offers the possibility of exploiting the curvature in H-storage technologies (5). We then studied increasingly hydrogenated graphene: we quantified the band gap opening as a function of H coverage, found in agreement with measurement (6), though with interesting exceptions for specific symmetries (Figure (c)). This opens the possibility of designing nano-electronics devices (7) by means of curvature controlled graphene hydrogenation.

The study with the complete model (>1600 atoms) also revealed that the substrate concurs in stabilizing one over two structures, equivalent as free standing layers, symmetric with respect to curvature inversion (8). In general, the control of curvature emerges as a key issue for graphene functionalization for high-tech applications. Therefore we are now exploring several strategies for rippling creation and manipulation. In the same study, we applied external electric fields orthogonal to the sheet and observed that the curvature is enhanced, and that the effect is increased in the presence of B/N substitutional doping (Figure (d)). This is the signature of a flexoelectric effect (8), which needs however further investigations. Other possible strategies for curvature control are the coupling to piezoelectric substrates or the functionalization with pillar molecules sensitive to external stimuli, which should also serve as spacers to create a 3D functional structure.

This work is also supported by EU, 7th FP, Graphene Flagship (contract no. NECT-ICT-604391).

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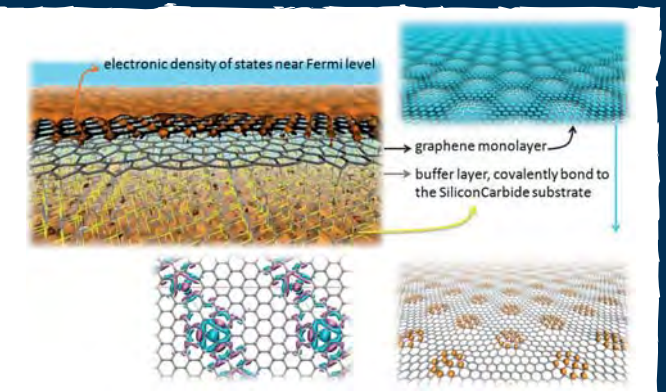
(a)

Figure (a) Optimized structure of graphene grown on SiC
Figure (b) Rippled free standing graphene monolayer
Figure (c) Ripples driven graphene hydrogenation
Figure (d) Electronic charge displacement in N/B substituted graphene



(b)

(c)

(d)

ISCRA

Numerical Simulations of Beam Driven Plasma Waves Using a Massively Parallel 3D ALaDyn-PIC code

The project has been designed to perform parallel 3D particle-in-cell (PIC) simulations of electron acceleration by a plasma wakefield, using the ALaDyn code [C. Benedetti et al., IEEE Transaction on Plasma Science 36,1790 (2008) and P. Londrillo et. al Nucl. Inst. and Meth. A 620 (2010) 28].

The simulation investigation refers to the physical regime where one or more electron bunches injected on a pre-ionized plasma drive a wake (PWFA) characterised by field gradients orders of magnitude higher than those obtained with traditional accelerating cavities.

In particular, we are interested in reproducing the experimental conditions of the COMB experiment in preparation at Sparc_Lab [M. Ferrario et al., Nucl.Instr.Meth. B 309, 183 (2013)], a facility at the National Laboratory of Frascati of INFN. Here, a train of low-emittance electron-bunches of about 100-150 MeV energy will enter a channel of pre-ionised plasma confined by a capillary tube. The front bunch(es), acting as drivers, will yield energy to the plasma creating the field that will accelerate the last beam of the train, called 'witness'. A simulation example, obtained with ALaDyn, containing a single driver followed by a witness, is shown by a 2D slice in the first figure (Fig.1), and in a fully 3D rendering in figure (Fig.3).

The goal of the simulation is to find the best experimental configuration needed to obtain the highest witness-beam acceleration and quality, keeping the emittance and the energy spread as close as possible to the typical values achieved with the Sparc linac.

We investigated several experimental configurations both in linear and non-linear regimes, using schemes with single or multiple drivers. Of particular interest is the quasi non-linear regime [J.B. Rosenzweig et al. Phys.Rev. Special Topics 7, 061302 (2004)], where the plasma response is still linear (the field adds up linearly) but a small blow-out region, typical of the non-linear regime, is created around the witness. The linear profile of the longitudinal and transverse fields, created inside the blow-out region, is suitable for minimizing emittance growth of the beams. An example is given in figure (Fig.2) where transverse (red line) and logitudinal (blue line) fields are shown as a function of the transverse coordinate as obtained from a simulation in the quasi non-linear regime with three drivers. These results where published in [Londrillo, P. and Gatti, C. and Ferrario, M. "Numerical investigation of beam-driven PWFA in quasi-nonlinear regime", Nucl.Instrum.Meth. A740 236-241 (2014)].

We will perform further studies on the transverse and longitudinal dynamics of the beams in order to understand the best matching conditions for their injection and propagation in the plasma and we did a systematic comparison of simulation results with theoretical expectations from envelope equations.

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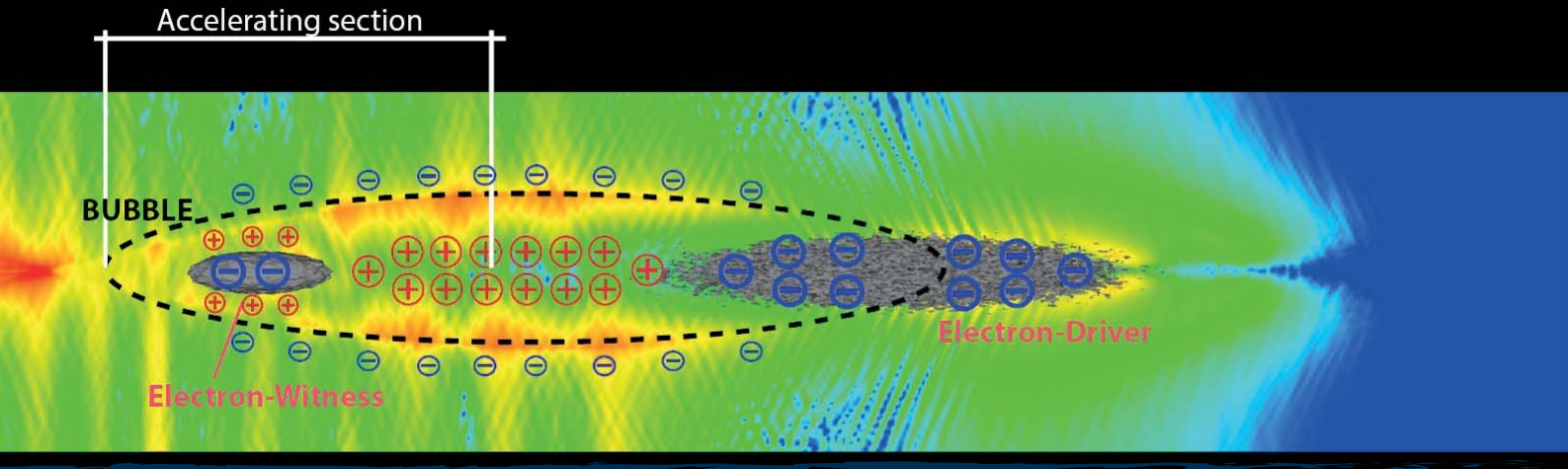

Figure 1: A 3D plot of the electric fields intensity with overlapped the density of two relativistic electron bunches: on the right the main bunch driving a wake of intense plasma waves, on the left a witness bunch to be accelerated by the wake longitudinal electric field . A superposed cartoon of positive and negative charges of the wake helps to illustrate some dynamical aspects.

Figure 2: This image like the previous one highlights the electric field structure, overexposed to the bunch positions to visualize the relative position of the electric field with respect to the bunch. The image, seen from the side highlights the 3D nature of the calculation and the bubble shape. The 3D contour plot easily show to the reader the particular corrugated nature both of the driver and of the witness (bunch ahead and following bunch respectively). At this distance: about 1.5 cm in a capillary gas, the density contour plot highlights how the driver begins to deplete, and how the witness begins to become unstable denoting a kinetic sausage like instability profile.

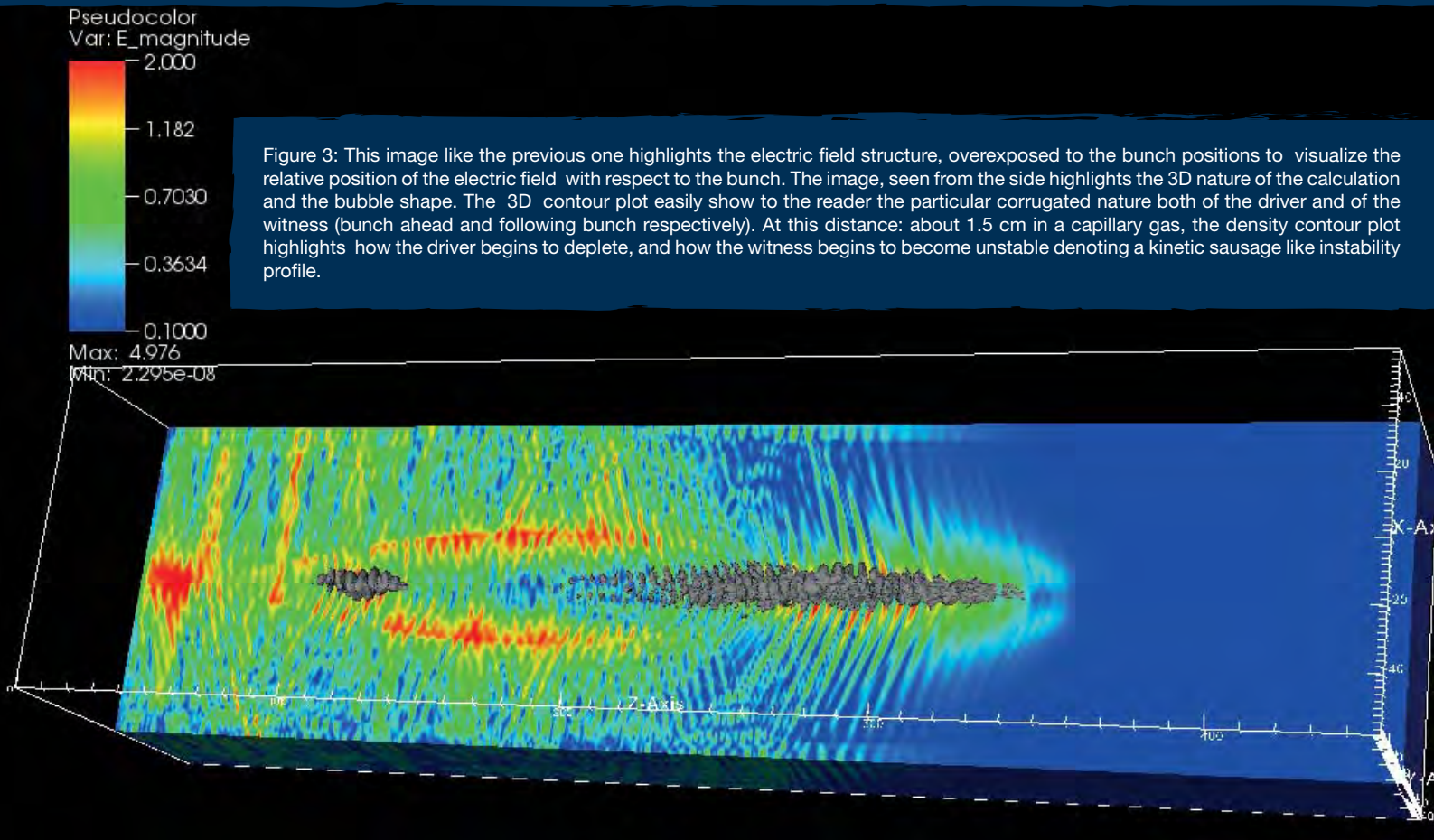

Figure 3: This image like the previous one highlights the electric field structure, overexposed to the bunch positions to visualize the relative position of the electric field with respect to the bunch. The image, seen from the side highlights the 3D nature of the calculation and the bubble shape. The 3D contour plot easily show to the reader the particular corrugated nature both of the driver and of the witness (bunch ahead and following bunch respectively). At this distance: about 1.5 cm in a capillary gas, the density contour plot highlights how the driver begins to deplete, and how the witness begins to become unstable denoting a kinetic sausage like instability profile.

ISCRA

SPATIAL - SPectral-element and Adjoint 3D full-wave Tomography for ItALy

The principal breakthrough of our project is to obtain a comprehensive 3D velocity model for Italy at unprecedented high frequencies (up to ~0.2 Hz) and constrained by full observed seismic waveforms, that can be considered as the reference model for this region. This paramount task has never been done nor even been feasible before because it requires using simultaneously the recorded data of modern and dense seismological networks, a strong and efficient numerical approach and an enormous computational power only recently made available through the resources of advanced national and international HPC centres.

We plan to exploit the powerful combination between the Spectral-Element Method (SEM, code SPECFEM3D) for the numerical simulation of seismic wavefields (e.g., Peter et al., 2011) and the adjoint methods for the tomographic inversion (e.g., Tape et al., 2009) in order to solve large scale inverse problems. The SEM is a well-established approach for accurately modelling seismic wave propagation in realistic 3D heterogeneous media and complex earthquake sources, boasting high computational efficiency and exponential accuracy. The adjoint technique is an inversion strategy that is able to exploit the differences between full observed and synthetic waveforms in order to illuminate the 3D sensitivity to model perturbations, reflected by so-called sensitivity kernels, and to iteratively improve fully 3D initial models.

Our project applies this innovative and successful procedure for the first time to the whole Italian region (i.e., the whole country plus its surroundings), focusing a crucial point of its mission on the worldwide common urgency of increasing the resolution of Earth interior imaging. In turn, having as principal aim to create a very accurate velocity model of Italy makes our project very timely in order to enhance the capability in reliably reproducing seismic ground motion for very complex structures and seismic sources. This is a paramount task, not just in seismology but also for the civil community, in view of predicting large earthquake ground motion and assessing seismic hazard, especially in a country such as Italy affected by relevant seismicity and frequently struck by destructive events. Thus, the goals of this project will also help to address important societal issues. The new reference 3D model will yield precious contributions to the construction of ground shaking maps, resulting in a strong impact also for engineering purposes and for planning effective preventive measures based on rapid, reliable hazard scenarios. Another important point of novelty is that our project also involves refinements of seismic source solutions based on 3D velocity models, offering the unprecedented opportunity to create an updated catalogue of the seismic sources of Italian earthquakes also for small events (magnitude < 3).

We would like to thank the ISCRA program for allowing us to exploit the Cineca high-performance computing resources. This enables us to perform a first important step towards the realization of the ambitious project in computational seismology of obtaining a new reference 3D velocity model for the whole Italian region. Results of this project are very useful as preparatory phase for our larger PRACE project recently awarded.

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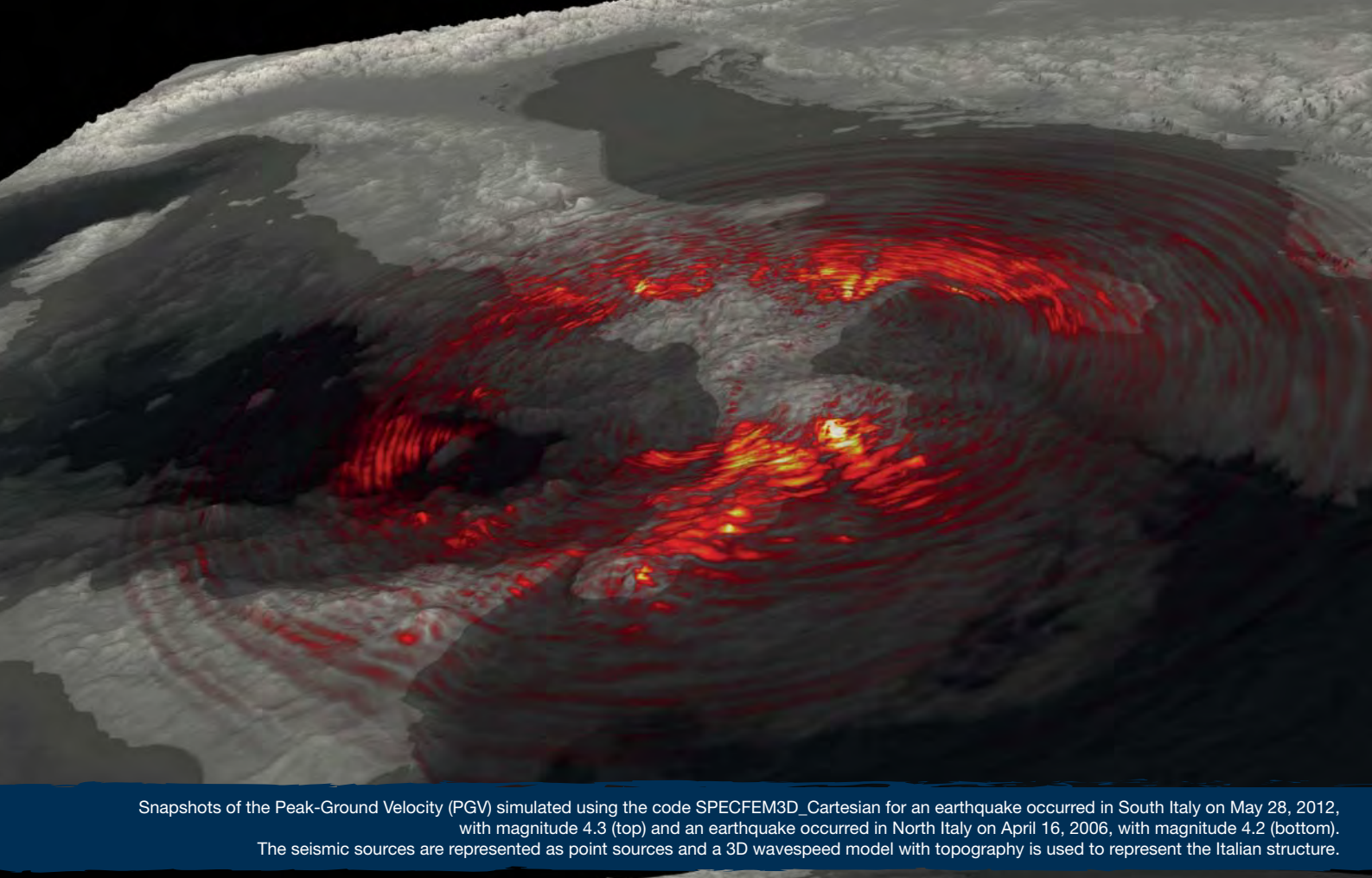
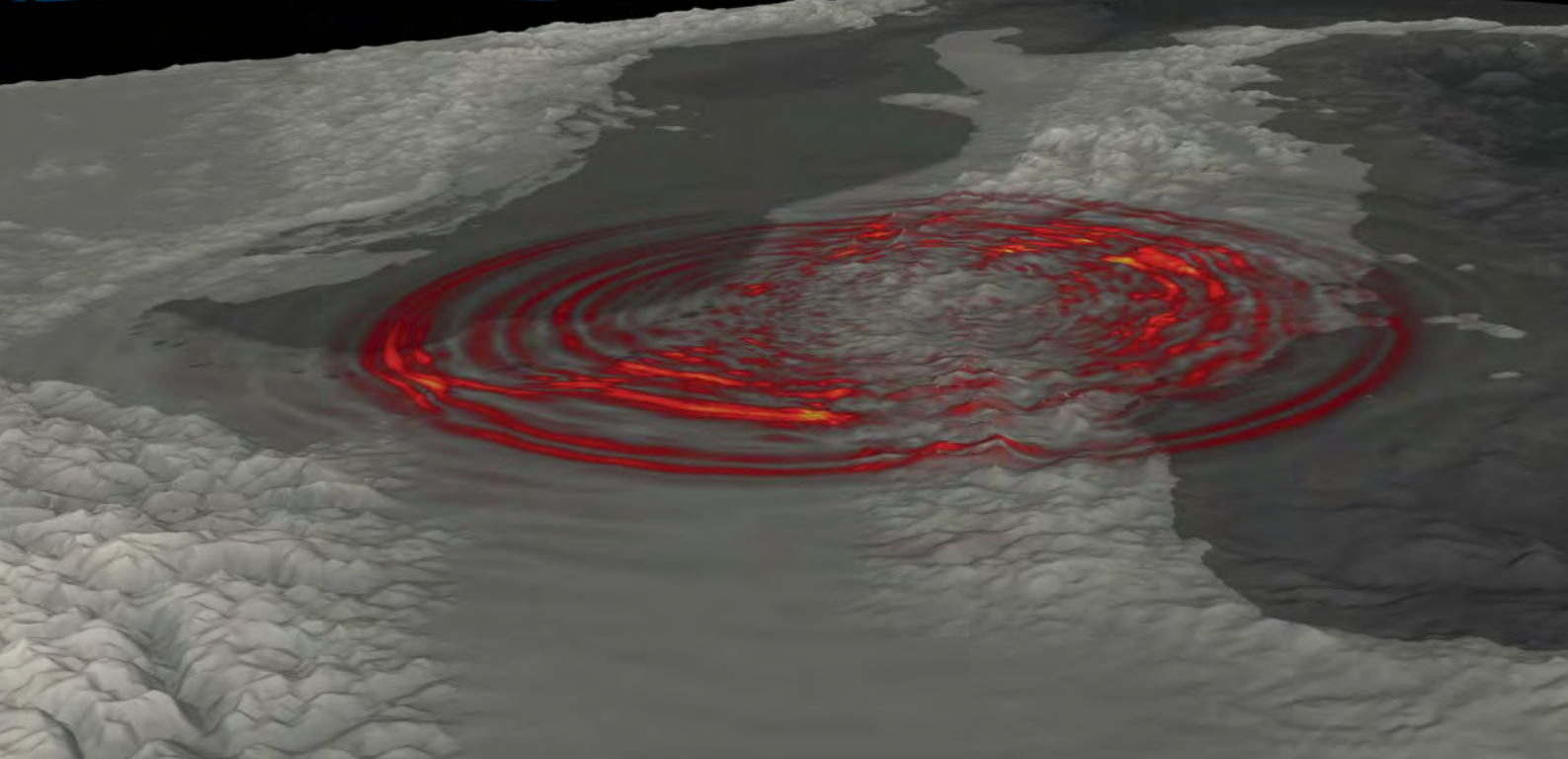


Snapshots of the Peak-Ground Velocity (PGV) simulated using the code SPECFEM3D_Cartesian for an earthquake occurred in South Italy on May 28, 2012, with magnitude 4.3 (top) and an earthquake occurred in North Italy on April 16, 2006, with magnitude 4.2 (bottom).
The seismic sources are represented as point sources and a 3D wavespeed model with topography is used to represent the Italian structure.



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Multiexcitons at a Cost of One: Carrier Multiplication in Silicon Nanocrystals

The realization of nano-structured third generation solar cell devices is a fundamental step in order to significantly increase the percentage of electrical energy generated by photovoltaic modules. In these systems the possibility to manipulate optoelectronic properties by nanocrystal size reduction and to exploit new recombination and relaxation mechanisms can increase the percentage of sunlight frequencies available for energy conversion and lead to a large use of the excess energy. In particular, high-energy loss factors can be minimized promoting fast and non-dissipative recombination mechanisms like for instance the Carrier Multiplication (CM) effect. CM is a Coulomb driven relaxation process that results in the generation of multiple electron-hole pairs after absorption of a single photon. In this process a highly excites carrier (initial carrier) decays toward the band edge and excites (at least) one valence electron across the bandgap, thus producing additional e-h pairs. At the nanoscale, CM can be as fast as or even faster than other radiative and non-radiative competitive recombination processes (phonon scattering, Auger cooling and direct radiative recombination). CM represents therefore an effective way to minimize energy loss factors and therefore a possible route to increase solar cell photocurrent and hence solar cell efficiency. By adopting a like-chain combination of codes based on both the Density Functional Theory DFT (pw-scf, QUANTUM Espresso package) and the Density Functional Perturbation Theory DFPT (DBS code), we have calculated CM lifetimes by applying first order perturbation theory to Kohn-Sham states (RECOMB code). We have analyzed CM dynamics considering systems of isolated and strongly interacting silicon nanocrystals Si-NCs ($Si_{35}H_{36}$, $Si_{147}H_{100}$, $Si_{293}H_{172}$, $Si_{87}(OH)_{76}$, $Si_{147}(OH)_{100}$, $Si_{147}H_{100}$ x $Si_{293}H_{172}$), with a size ranging from 1.3 to 2.5 nm.

In particular we have clarified:

1) The role played by quantum confinement on CM dynamics.

When isolated NCs are considered, CM lifetimes decrease when the energy of the initial carrier Ei increase. At low energies, CM is more efficient in large NCs due to their low energy gap (and therefore low CM energy threshold). At the contrary, at high energies, CM is almost size independent. At low energies CM lifetimes shows strong fluctuations.

This effect is induced by the strong discretization of the NCs electronic state near the valence and conduction band edges that produce a scattering among different order of magnitude of the effective coulomb matrix elements. At high energies, instead, effective coulomb matrix elements stabilize on a constant value that depend only on the NC size. In this portion of energies, therefore the typical trend of the CM lifetimes, that decrease with Ei, is only connected to the monotonically increasing behavior of the density of the final states [1].

2) The role played by NCs interplay on CM dynamics.

We have investigated effects induced by NCs interplay on CM effects by considering systems formed by two different Si-NCs (see Fig. 2). We have proven that NCs interaction intensifies CM dynamics at low energies, thus leading to a red-shift of the CM energy threshold. This effect is very important and can extend the possibility to exploit CM recombination effects to improve solar cell performances. At the contrary, at high energies, NC-NC interaction only weakly modifies CM efficiency [2]. In these conditions systems of closely packed NCs behave like sparse arrays of non-interacting NCs.

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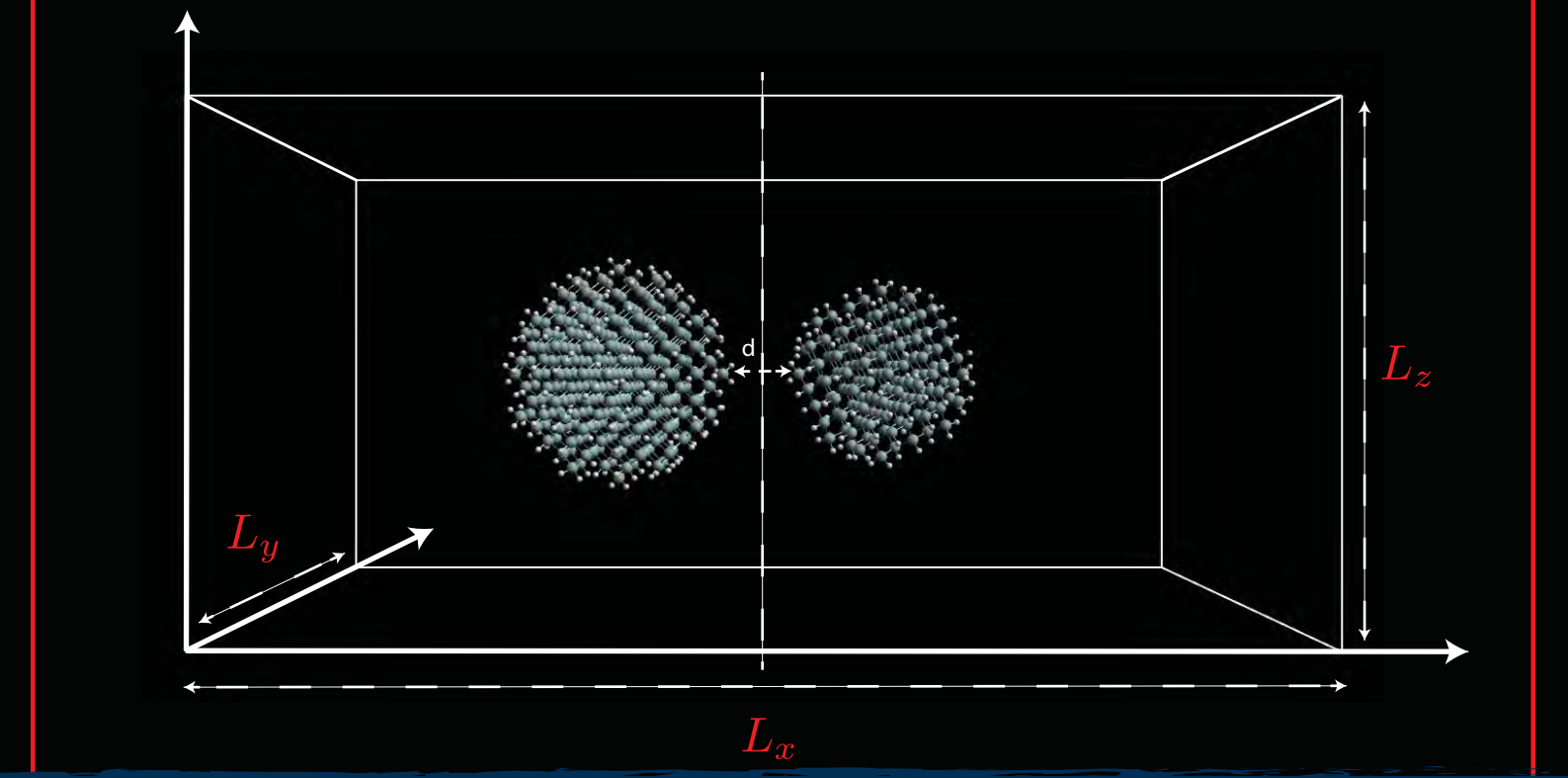
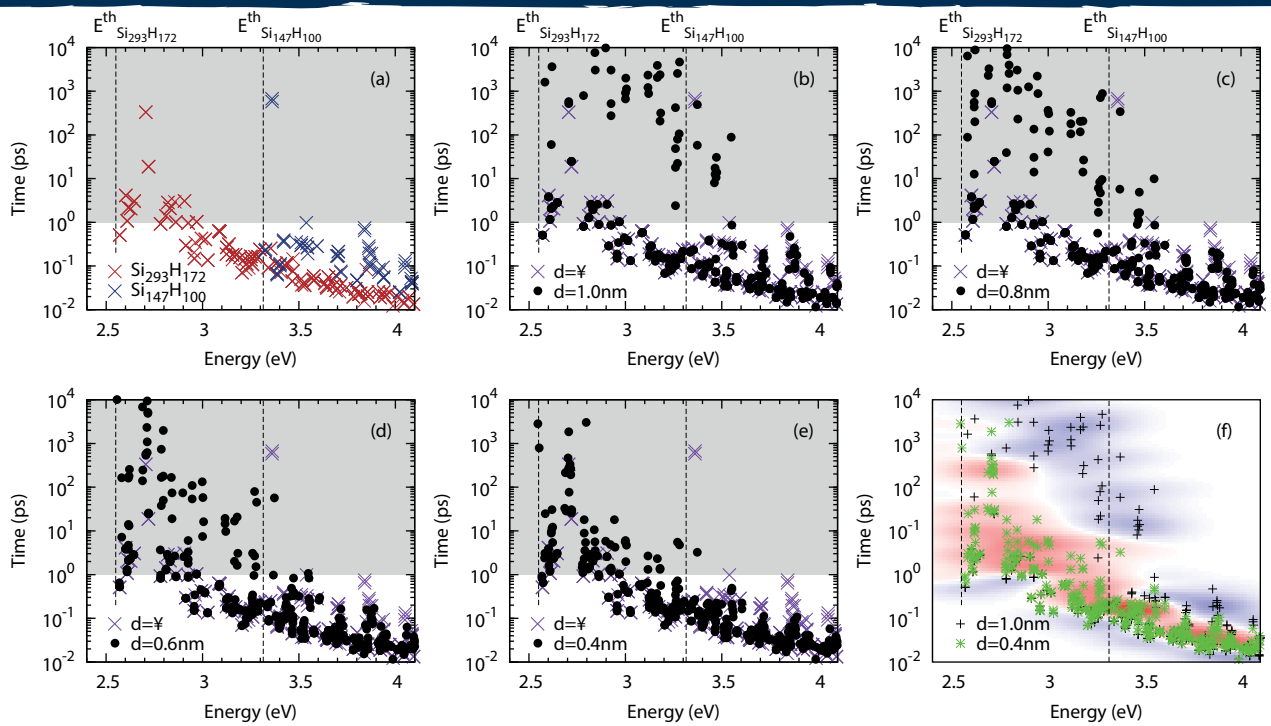


Figure 1: The simulation box for the system $Si_{293}H_{172}$ X $Si_{147}H_{100}$ is reported in the figure. Lx = 10 nm Ly = 4.8 nm and Lz = 4.8 nm. The $Si_{293}H_{172}$ is placed on the left part of the cell while the Si147H100 is placed on the right part of the cell. The vertical dashed plane divides the box in two identical parts. Reprinted from I. Marri et al., J. Am. Chem. Soc. 136, 1327 (2014). Copyright 2014 ACS.

Figure 2: Calculated CM lifetimes for the system $Si_{293}H_{172}$ X $Si_{147}H_{100}$ are reported as a function of the NC-NC separation and of Ei. NCs have a diameter ofabout 2.4 and 1.9 nm and an energy gap of 1.70 and 2.21 eV, respectively. In panel (a), NC-NC interaction is turned off. Red (blue) crosses identify calculated CM lifetimes for the isolated $Si_{293}H_{172}$ ($Si_{147}H_{100}$). From panel (b) to panel (e) calculated CM lifetimes are reported considering NC-NC separation ranging from 1.0 to 0.4 nm (black points). Purple crosses keep track of the CM lifetimes calculated for isolated Si-NCs. The difference between distributions calculated in panels (e) and (b) are reported in panel (f). Here red (blue) zone point out an intensification (reduction) of the CM efficiency. Reprinted from I. Marri et al., J. Am. Chem. Soc. 136, 1327 (2014). Copyright 2014 ACS.



ISCRA

Filling the gap between supernova explosions and their remnants

Supernova remnants (SNRs), the leftovers of supernova (SN) explosions, are diffuse extended sources with a quite complex morphology not completely understood. General consensus is that this morphology reflects the physical and chemical properties of the SN from which the remnant arises. Thus filling the gap between SN explosions and their remnants is very important in Astrophysics for a comprehension of the origin of present-day structure of SNRs and to probe and constraint current models of SN explosions. A detailed model connecting the SN explosion with the SNR evolution is presently missing.

In the framework of a PRACE project (N.2012060993) and an ISCRA class B project (N.HP10BI36DG,2012) we developed a model describing the dynamics of the stellar ejecta formed during the SN outburst from the immediate aftermath of the SN explosion to their expansion in the SNR with unprecedented model resolution and completeness. The aim was to answer, for the first time, important questions as: how does the final remnant morphology reflects the inner mechanisms of the SN engine?

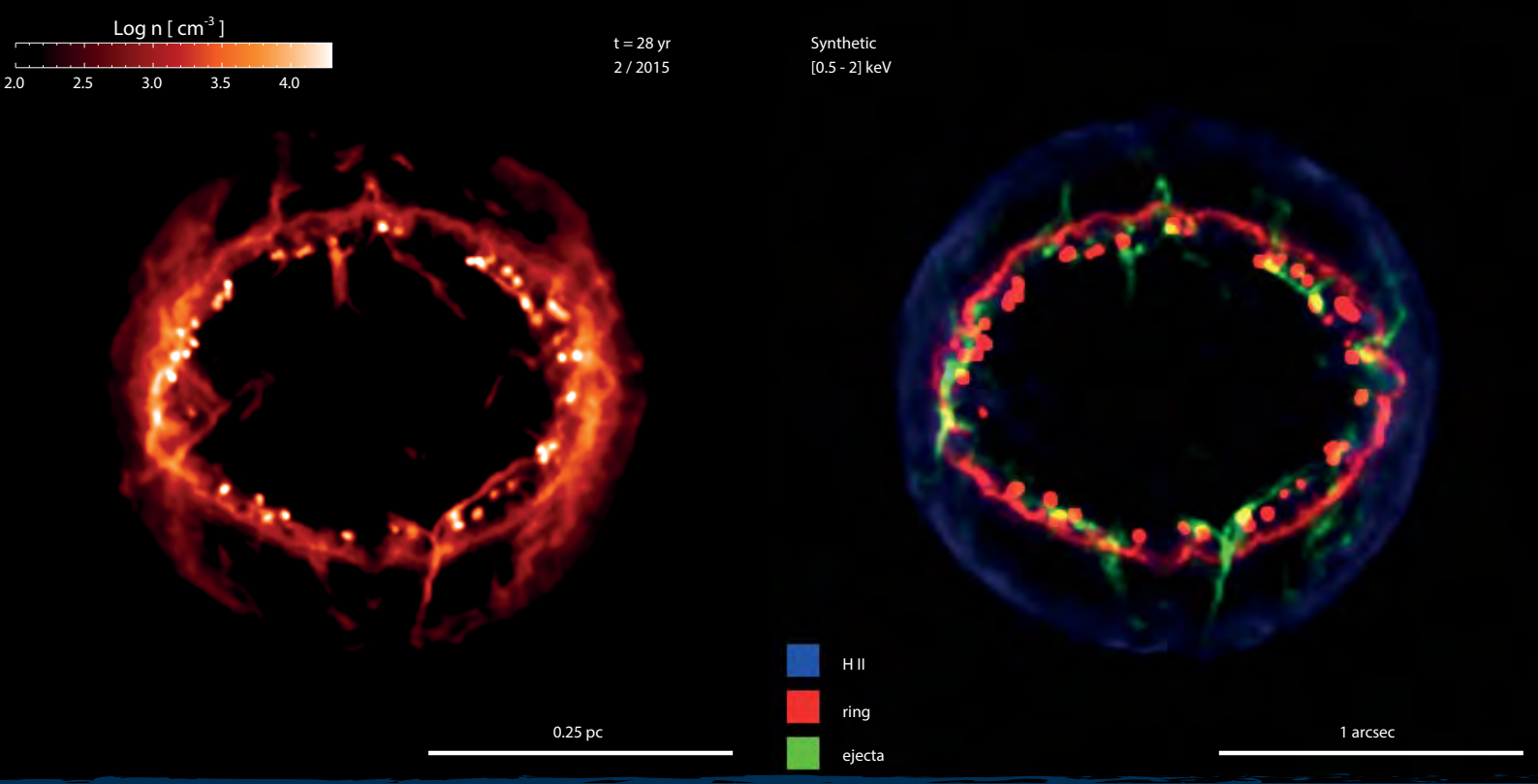
The simulations have been tuned on two well studied core-collapse SNRs, namely Cassiopeia A and SN 1987A. In particular, because of its youth and proximity, SN 1987A is an ideal template to study the link between a SN and its remnant: it shows the transition of a SN into a SNR and offers the unique opportunity to link the morphological properties of the remnant to the inner mechanisms of the progenitor SN. For this study, we performed high-resolution hydrodynamic simulations describing the post-explosion evolution of the SN and the following three-dimensional interaction of its remnant with the surrounding nebula.

The comparison of model results with observations allowed us to disentangle the imprint of the SN on the subsequent remnant evolution (by constraining its energy and the mass of ejecta) from the interaction of the remnant with the nebula. Also the model enabled us to unveil the physical origin of the multicomponent plasma emission currently observed in X-rays. Finally, we showed that, in the next few years, the X-ray emission will be dominated by shocked ejecta and this will provide important clues on the dynamics of the explosion.

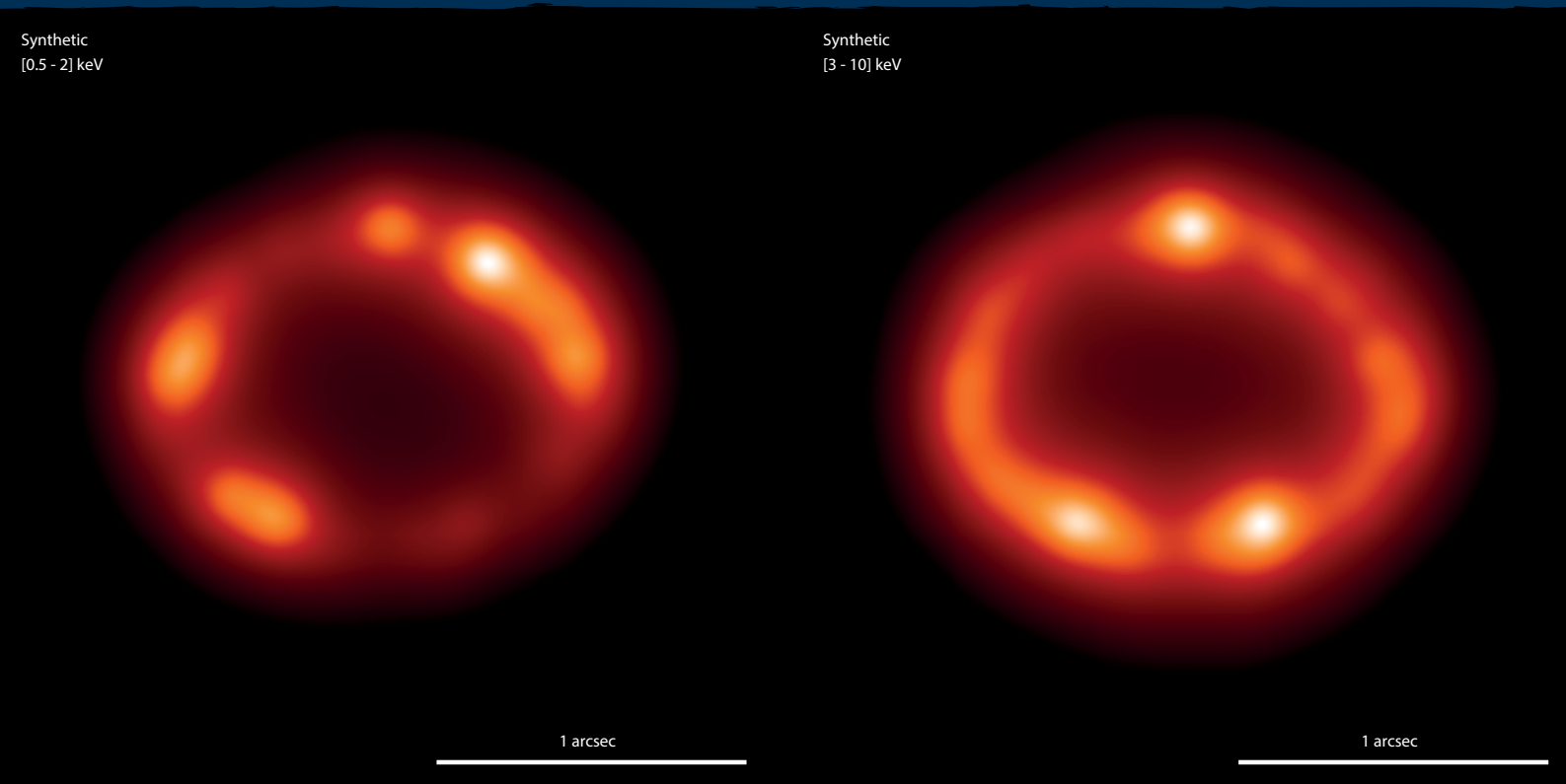
Salvatore Orlando, Fabrizio Bocchino
INAF - Palermo Astronomical Observatory

Marco Miceli, Fabio Reale, Giovanni Peres
Palermo University / INAF - Palermo Astronomical Observatory

Maria Letizia Pumo
INAF - Padova/Asiago Astronomical Observatory



Interaction of the blast wave with the surrounding nebula. Upper left: 3D volume rendering of particle density of the shocked plasma 28 years after the SN xplosion. Upper right: corresponding 3-color composite image of the X-ray emission integrated along the line of sight. The image is smoothed with a Gaussian of size 0.025 arcsec. The different colors in the composite show the contribution to emission from the different shocked plasma components, namely the ejecta (green), the ring (red), and the H\,II region (blue). Lower panels: synthetic maps of X-ray emission in the soft (on the left) and hard (on the right) X-ray bands integrated along the line of sight and smoothed to approximate the spatial resolution of Chandra observations.

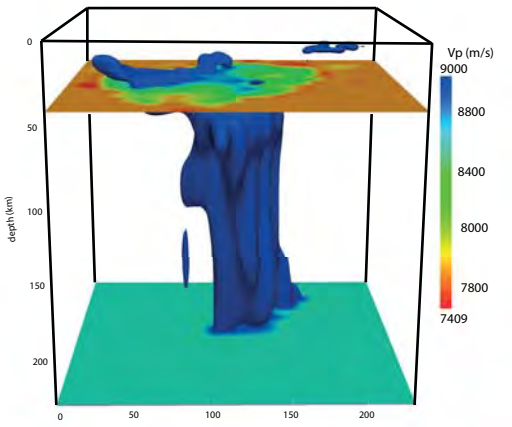


ISCRA

Full waveform tomography of the Vrancea region with a local dataset

Julie Baron
INGV

The study, part of a Ph.D, aims to improve the tomographic model of the Vrancea region in Romania, by adding more details to its seismic velocities distributions.
The main concept under tomographic inversion is to retrieve physical Earth parameters distribution from seismic signals, registered at seismic stations. The model updating is based on the discrepancies between observed waveforms signals and synthetic ones, computed in an a-priori Earth's model.
Here, the tomography is done by implementing a "full-waveform" inversion that allows retrieving as much information as possible from the seismic signals. The computation of the synthetics is done on Blue Gene/Q with the SPECFEM3D software that uses the spectral element method to solve the seismic waves equation in an heterogeneous hexahedral mesh. The model updating is based on a travel-time misfit criteria and follows a steepest descent minimization algorithm.
The database is composed of local seismic traces from the six months CALIXTO 1999 temporary experiment. The high noise level of the traces imposes to work in a relatively narrow high frequency band: between 1,25 and 2,5 seconds period. This leads to a high computational cost for the inversion workflow.
Ten model updates have been designed under this B project, allowing to dress preliminary results on the inversion method and workflow. Other iterations are necessary to be able to discuss and interpret a new Vrancea tomographic model.



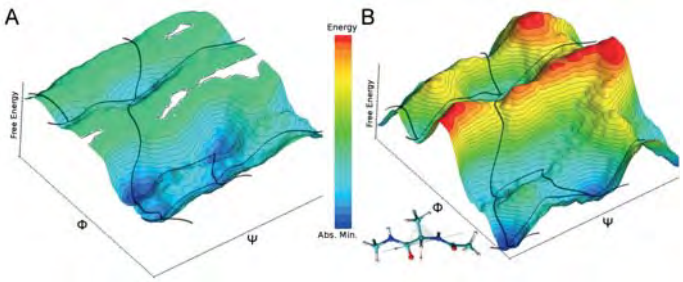
P velocity distribution (in m/s) of the initial model in a 3D view. The downgoing shape of the high velocity distribution is characteristic of the Vrancea seismic velocity distribution.

Probing conformations of peptides at gold/water interface: the first step to study how metal surfaces affect the protein folding

Luca Bellucci
S3, CNR NANO

Proteins and peptides have complex free-energy landscapes that determine their stable structure(s) and are also pivotal to their structural transformations, i.e., to their function. Interaction with inorganic surfaces and nanoparticles may affect such free energy landscape. Here, by means of large scale classical MD simulations, we show that the interaction with a metal surface is able to change the free-energy surface (FES) of the simplest peptide (alanine dipeptide) at the topological level (i.e., changing the qualitative appearance of the landscape), and we characterize the consequences of these changes in the peptide conformational ensemble. This result opens the way to rationalize at the atomic level the effects of metal surfaces and nanoparticles on the structure and function of peptides and proteins [1].

[1] Luca Bellucci and Stefano Corni, J. Phys. Chem. C 118 (2014)



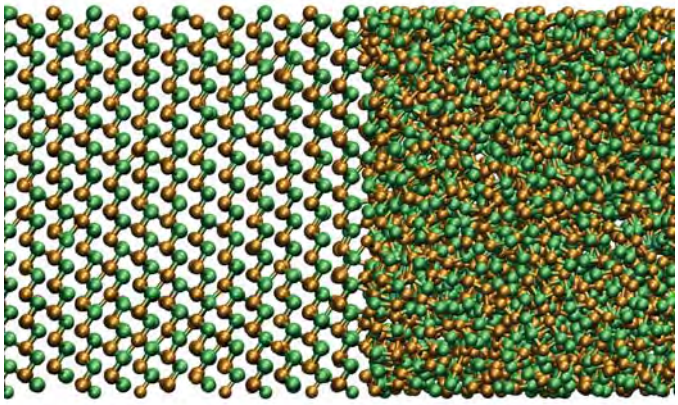
A. FES of the alanine dipeptide along Ramchandran angles in solution, far from the gold surface.
B. FES of the alanine dipeptide at the gold-water interface.

ISCRA

Atomistic simulations of thermal conductivity in phase change materials

Marco Bernasconi
Milano University

Chalcogenide alloys are of interest for their use in novel non volatile memories named phase change memories (PCM) which rest on a fast and reversible transformation between the amorphous and crystalline phases upon Joule heating. The thermal boundary resistance (TBR) at the interface between the chalcogenide and the surrounding dielectrics/electrodes is a crucial parameter for the control of thermal cross-talks with adjacent cell. Since the amorphous region is embedded in a crystalline, untransformed matrix, the junction between the crystal and the amorphous phases is another interface expected to affect the operation of the device. In this project, we performed large scale non-equilibrium molecular dynamics simulations on the phase change compound GeTe to estimate the TBR at the amorphous-crystal interface. The interatomic potential was generated by fitting with a Neural Network method a huge database of energies computed within Density Functional Theory. Moreover, an electronic contribution to the TBR arises due to energy transfer between electrons and phonons in the crystalline phase which was also computed from DFT phonons and electron-phonon coupling. The resulting total TBR (7 m^2K/GW) is comparable to the TBR at the interfaces with the surrounding dielectrics/electrodes and it must thus be included in a full electrothermal modelling of the device. The simulations have also shown that the linear response regime for thermal conductivity still holds at the extreme conditions of operation of the device where thermal gradients as large as 30 K/nm can be present.

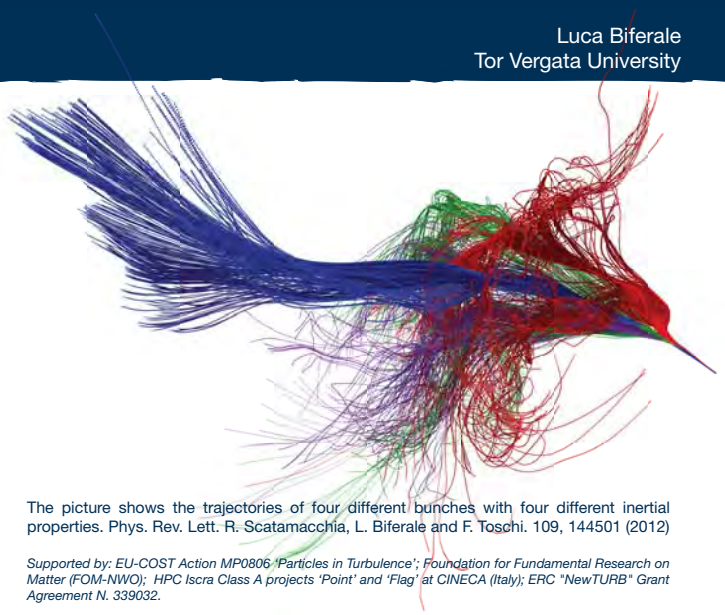


Snapshot of the slab model (22000 atoms) of the amorphous/crystal interface of the phase change compound GeTe. The model was used to compute the thermal boundary resistance and non-linear effects in thermal transport by means of non-equilibrium molecular dynamics simulations with a Neural Network interatomic potential.

Dispersion of particles in a turbulent flow

Luca Biferale
Tor Vergata University

Results from direct numerical simulations (DNS) of particle relative dispersion in three-dimensional homogeneous and isotropic turbulence at Reynolds number $Re \sim 300$ have been obtained. Simulations have been performed using state-of-the-art pseudospectral code at 1024^3 resolution. We have studied point-like passive tracers and heavy particles. Particles are emitted from localised sources, in bunches of thousands, periodically in time, allowing an unprecedented statistical accuracy. Statistics from single missions from single sources or from multiple emissions from multiple sources can be extracted. We have studied intense rare events characterising both extremely fast and slow separations. The right tail of the probability density function (PDF) for tracers develops a clear deviation from Richardson's self-similar prediction, pointing to the intermittent nature of the dispersion process. In our numerical experiment, such deviations are manifest once the probability to measure an event becomes of the order of – or rarer than – one part over one million, hence the crucial importance of a large dataset, as the one obtained in this project. The role of finite-Reynolds-number effects and the related fluctuations when pair separations cross the boundary between viscous and inertial range scales are also discussed. For the first time, we show that an asymptotic prediction based on the multifractal theory for inertial range intermittency and valid for large Reynolds numbers agrees with the data better than the Richardson theory. By using the exit-time statistics we also show that events associated with pairs experiencing unusually slow inertial range separations have a non-self-similar PDF.



The picture shows the trajectories of four different bunches with four different inertial properties. Phys. Rev. Lett. R. Scatamacchia, L. Biferale and F. Toschi. 109, 144501 (2012)

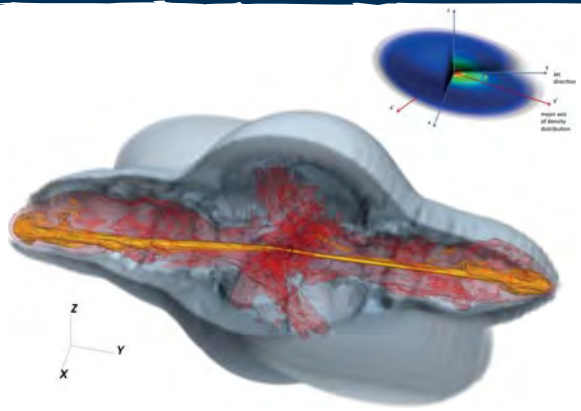
Supported by: EU-COST Action MP0806 'Particles in Turbulence'; Foundation for Fundamental Research on Matter (FOM-NWO); HPC Iscra Class A projects 'Point' and 'Flag' at CINECA (Italy); ERC "NewTURB" Grant Agreement N. 339032.

ISCRA

The origin X-shaped radiogalaxies

Gianluigi Bodo
INAF

Some of active galactic nuclei produce powerful relativistic jets that propagate to distance of up to 1Mpc and give origin to extended lobes of radio emission. These radiogalaxies are divided in two big classes depending on their power and morphology: Fanaroff-Riley I (FRI, less powerful) and II (FRII, more powerful). Among FRII, X-shaped radiogalaxies show, in addition to the normal lobes of emission, two additional low brightness wings forming an angle with the principal lobes. In order to understand the origin of this class of extragalactic radiosources, we simulated two relativistic magnetized jets, propagating in opposite directions in a triaxial ellipsoidally stratified medium, representing the galactic gas distribution. The jets are less dense than the surrounding medium and propagate close to the major axis of the ellipsoid. They excavate a cavity in the galactic gas and the colliding backflows, coming from the jet heads, escape along the minor axes of the ellipsoidal distribution forming wings similar to those observed in X-shaped radiogalaxies. We explored several combinations of jet parameters for understanding under which conditions this kind of structures can be formed and we showed that they are the result of jets with relatively low power (close to the separation between FRI and FRII) propagating in highly elliptical galaxies.

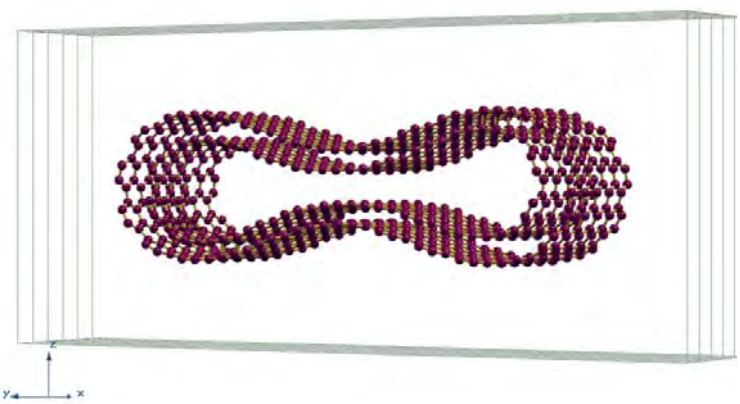


The figure shows the density distribution (in grey) of the external medium, together with the jet velocity distribution (in yellow-red). We can see the cavity formed by the jet and the wings escaping along the minor axes of the ellipsoid. In the upper right corner we show also the initial density distribution with a sketch of the geometrical setup. We can see that, in the present case, the jet propagates at an angle of 30° with the major axis of the ellipsoid.

Folded Graphene Multilayers

Cristian Degli Esposti Boschi
CNR-IMM

The general objective was to perform quantitatively accurate and realistic simulations at the quantum level (via DFT) of folded graphene sheets.
More specifically we aim to compute the charge and local dipoles redistributions in the proximity of folded graphene edges and their effects on the Transmission Electron Microscopy response so to carry out a detailed comparison. Reported data suggest the valence charge redistribution at the surfaces to be at the basis of the unusual properties of these materials, that eventually can be functionalized selectively according to such a behaviour.
The most demanding step is the relaxation of the starting atomic configurations towards the minimum-energy arrangement. Once this has been properly done, the structural information, such as strain, and charge or potential fields can be computed on a spatial grid well below the current experimental resolution.
The simulations are made with the Quantum Espresso suite that employs periodic boundary conditions. Hence, in order to reconstruct a folded edge, one is led to consider a configuration as shown in the figure. Physically, it is necessary that the central adhesion region is sufficiently large so that the contribution from non-bonding interactions compensates the elastic energy that leads the folded membranes to open. In particular we have employed the so-called VDW-DF2 exchange-correlation scheme to describe the van der Waals interactions at the DFT level and obtain the relaxed multilayer membranes with different fold orientation (chirality) up to some hundreds of atoms.



Repeated supercell containing 192 carbon atoms used for the simulation of two-graphene-layers folded edge.

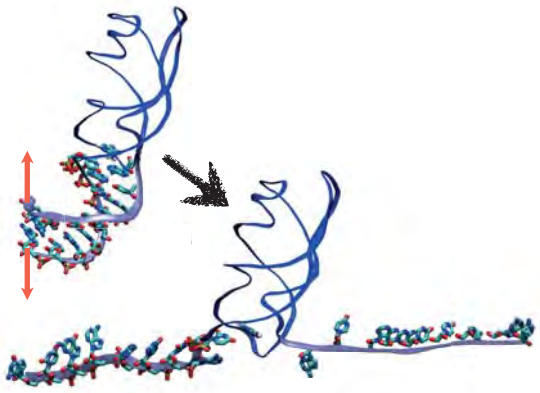
ISCRA

Conformational transitions in the adenine sensing riboswitch

Giovanni Bussi
SISSA

Riboswitches are structured mRNA elements that modulate gene expression. They undergo conformational changes triggered by highly specific interactions with sensed metabolites. Among the structural rearrangements engaged by riboswitches, the forming and melting of the aptamer terminal helix, the so-called P1 stem, is essential for genetic control. The structural mechanisms by which this conformational change is modulated upon ligand binding mostly remain to be elucidated. We here used massively parallel pulling molecular dynamics simulations to study the thermodynamics of the P1 stem in the add adenine riboswitch. The P1 ligand-dependent stabilization was quantified and compared with thermodynamic data. This comparison suggests a model for the aptamer folding in which direct P1-ligand interactions play a minor role on the conformational switch when compared with those related to the ligand-induced aptamer preorganization [1].

[1] Di Palma, Colizzi, and Bussi, RNA 2013, 19, 1517

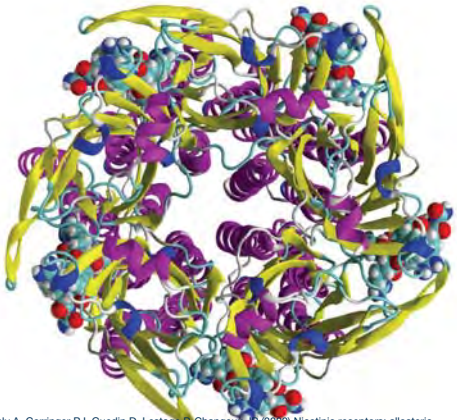


Structure of the adenine riboswitch aptamer before and after pulling its end-to-end distance. Pulled directions are indicated by red arrows. Figure adapted from [1].

Large scale motions in models of human nicotinic receptors

Grazia Cottone
Palermo University

Nicotinic acetylcholine receptors (nAChRs) are involved in many biological processes [1] and are implicated in the onset of Alzheimer's disease and nicotine addiction [2]. The channel pore in the transmembrane domain (TMD) opens following the binding of agonists in the extracellular domain (LBD); the channel is closed when either no ligand is present or an antagonist is bound, and in the desensitized, agonist-bound state. Within this project, new chimeric models of the human $\alpha 7$ nAChR are generated, using the glutamate receptor (GluCL, [3]) as template for the TMD in the open state, and the AChBP protein [4] to model the LBD bound to the agonist *epibatidine* or to the antagonist *conotoxin* (see Figure). MD simulations of the fully solvated protein/membrane system complexed with *epibatidine* are run with NAMD2. A spontaneous collapse toward a non conductive channel is observed, irreversible on a 200 ns time scale. To sustain the open channel, a 200 ns simulation is run by applying a restraint on the hydrophobic rings that regulate the water passage in the channel. To further validate the obtained open conformation, four more 200 ns simulations are run, starting from configurations picked along the restrained trajectory, and by turning off the restraint. We therefore assess the stability of the putative open state over 1.0 μs cumulative simulation time. This work is the first one using GluCl as template for a human nAChR, providing a stable open form as demonstrated by i) the structural parameters describing the rigid-body motions of the TMD helices; ii) most importantly, the stationarity of the hydration level of the pore, fully corresponding to a conductive channel.



New homology model of human alpha7 nicotinic receptor generated by using the open TMD of the glutamate receptor (PDB entry: 3RIF) and the conotoxin-bound AChBP (PDB entry:2BYP) to model the LBD (top view). Conotoxin in vdw representation.

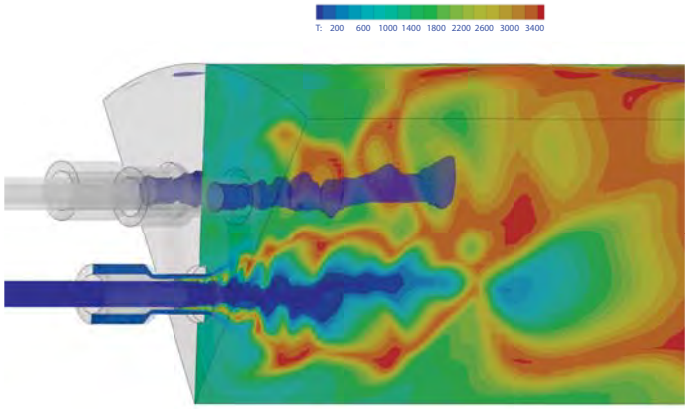
[1] Taly A, Corringer PJ, Guedin D, Lestage P, Changeux JP (2009) Nicotinic receptors: allosteric transitions and therapeutic targets in the nervous system. Nat Rev Drug Discov 8: 733-750
[2] Larsson A, Engel JA (2004) Neurochemical and behavioral studies on ethanol and nicotine interactions. Neurosci Biobehav Rev 27: 713-720
[3] Hibbs R E ad Gouax E (2011) Principles of activation and permeation in an anion-selective Cys-loop receptor. Nature 474: 54-60
[4] Hosseini Z, Malliavin T, Maragliano L, Cottone G, Ciccotti G (2014) Conformational Changes in Acetylcholine Binding Protein Investigated by Temperature Accelerated Molecular Dynamics. PLOS ONE e88555

ISCRA

Supercritical Combustion in Liquid Rocket Engines - temperature field

Francesco Creta
CIRA, La Sapienza University

Liquid Rocket Engines (LRE) technology is today in its full maturity although the complex phenomenology occurring within the thrust chamber is only partially understood. Recent trends show that the new challenges call for reliability and increasing performance of the rocket system, even with restricted budgets and shortened development time. In this framework the application of Computational Fluid Dynamics (CFD) is a key predictive tool for combustion chamber phenomena. Propellants are typically injected and burnt in a high pressure environment which can drive them to be in a supercritical thermodynamical state. In these conditions, molecular interactions affect significantly the fluid properties, so that a real gas equation of state and suitable relations for the transport properties become mandatory for a numerical simulation. A deeper insight into this phenomena is given by recent works on detailed simulation of trans- and supercritical flows by means of direct numerical simulations (DNS). Transition through super-criticality, together with chemical reactions and high turbulent levels implies spatial and temporal scales that make these processes impractical to be simulated directly. Reynolds-Averaged Navier-Stokes (RANS) and Large Eddies Simulation (LES) are therefore necessary to attempt numerical simulation on realistic length scales. The aim of a predictive CFD tool is to analyze the propellant injection into a rocket combustion chamber through multiple coaxial injectors and the subsequent combustion process. In this framework we carry out a series of RANS and LES simulations within an MPI (message passing interface) infrastructure in order to systematically validate real gas behavior in high pressure, chemically reactive turbulent flows.

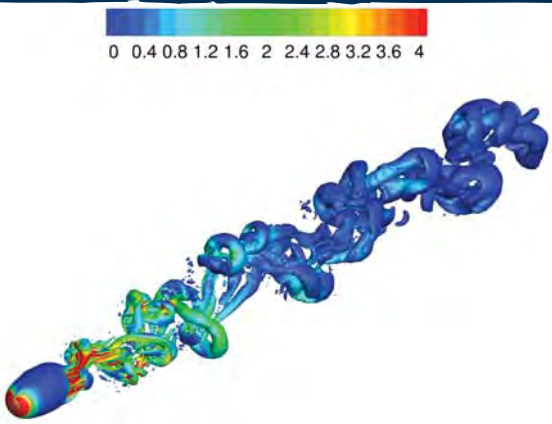


(A) At time t=0, the ions are separated from each other by a water wire consisting of 5 hydrogen bonds.
(B) Within less than 300 fs, the hydroxide ion quickly shuttles across three hydrogen bonds getting closer to the hydronium.
(C) In the next 100 fs, both the hydronium and hydroxide then find each other and undergo neutralization.

Assessment of a high-order Discontinuous Galerkin solver for DNS of the turbulent incompressible flow past a sphere

Andrea Crivellini
UNIVPM

This work deals with the assessment of a high-order discontinuous Galerkin (DG) incompressible solver, see for instance [1], for the Direct Numerical Simulation (DNS) of the massively separated flow past a sphere at Re = 1000. Indeed, at this flow regime, a transition to turbulence occurs in the wake region.
The employed DG method is fully implicit in time and its distinguishing feature is the formulation of the inviscid interface flux, which is based on the solution of the Riemann problem associated with a local artificial compressibility-like perturbation of the equations. The space discretized equations are integrated in time by means of high-order implicit time integration schemes, in order to exploit the benefits of high-order discretization both in space and time.
Moreover, the code is able to deal with unstructured hybrid grids, even consisting of curved elements, thus fully exploiting the well-known great geometrical flexibility, without compromising the high-order accuracy, proper of DG methods.
The computed solutions are fourth- and fifth-order accurate in space for pressure and velocity components, respectively, while are third-order accurate in time. The results are in very good agreement with the available literature data, thus demonstrating that DG methods are well suited to accurately address the DNS of turbulent flow, due to their good dissipation and dispersion properties. Moreover, this work demonstrated the reliability and stability of a high-order DG code in handling a really large number of degrees of freedom, up to about 8×10^6, on massively parallel architectures (up to 4096 FERMI cores).



Instantaneous λ_2 =0 iso-surface colored by non-dimensional vorticity magnitude

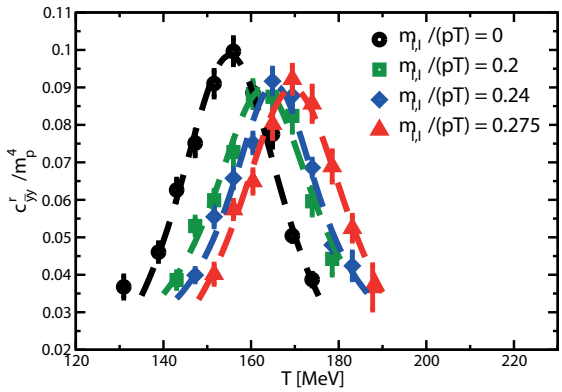
[1] Crivellini, A., D'Alessandro, V., Bassi, F., Assessment of a high-order discontinuous Galerkin method for incompressible three-dimensional Navier-Stokes equations: Benchmark results for the flow past a sphere up to Re=500, Computers and Fluids, 86, pp. 442-458, 2013

ISCRA

Exploring the Phase Diagram of Strongly Interacting Matter

Massimo D'Elia
Pisa University

The purpose of this project was that of making a steady step towards a full understanding of the phase diagram of strong interactions, something which is essential to correctly describe the early stages of the Universe, when a plasma of quarks and gluons was present, then transforming in ordinary hadronic matter, like the one we know today, at a pseudocritical temperature Tc.
Our aim was to determine, by lattice QCD simulations, how Tc depends on the baryon chemical potential muB, something which is relevant to a controlled reproduction of the same transition in high energy heavy ion experiments.
Numerical simulations at finite muB are hindered by the well known sign problem (the path integral measure is complex): to avoid that, we have implemented the method of analytic continuation from imaginary chemical potentials, applying it to a faithful discretization of Quantum Chromodynamics (QCD) with the three lightest families of quarks (up, down and strange). An intermediate result of our study has consisted in a better understanding of the phase diagram of the theory in the presence of imaginary chemical potentials.
As a final achievement, we have obtained a reliable determination of the curvature of the pseudocritical line and a critical comparison with previous results in the literature, aimed at reaching a full control over possible systematic effects. Results have been collected in a recent preprint, http://arXiv.org/abs/arXiv:1410.5758, that will be submitted for publication to a high impact scientific journal.

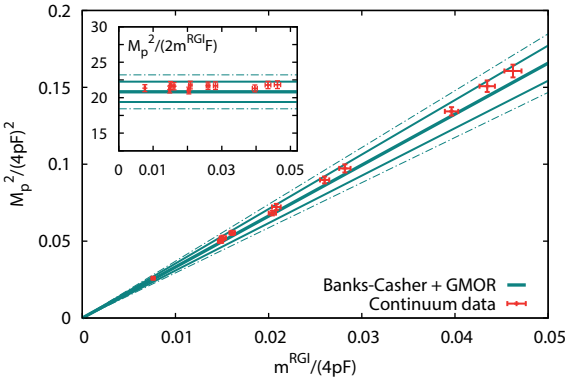


The figure shows the peak of the chiral susceptibility, signalling the chiral transition, as a function of the imaginary quark chemical potential. The displacement of the peak is used to obtain the curvature of the pseudocritical line by analytic continuation to real chemical potentials.

Chiral condensate for 2-flavor QCD

Georg Engel
Milano Bicocca University

A distinctive feature of the presence of spontaneous chiral symmetry breaking in QCD is the condensation of low modes of the Dirac operator near the origin. The rate of condensation must be equal to the slope of $M_\pi^2 F_\pi^2/2$ with respect to the quark mass m in the chiral limit, where M_π and F_π are the mass and the decay constant of the Nambu-Goldstone bosons. We compute the spectral density of the (Hermitian) Dirac operator, the quark mass, the pseudoscalar meson mass and decay constant by numerical simulations of lattice QCD with two light degenerate Wilson quarks. We use CLS lattices at three values of the lattice spacing in the range 0.05–0.08 fm, and for several quark masses corresponding to pseudoscalar mesons masses down to 190 MeV. Thanks to this coverage of parameters space, we can extrapolate all quantities to the chiral and continuum limits with confidence.
The results show that the low quark modes do condense in the continuum as expected by the Banks–Casher mechanism, and the rate of condensation agrees with the Gell–Mann-Oakes-Renner (GMOR) relation, as seen in the figure.
For the renormalisation-group-invariant ratios we obtain
$[\Sigma^{RGI}]^{1/3}/F = 2.77(2)(4)$ and $\Lambda^{MS}/F = 3.6(2)$, which correspond to
$[\Sigma^{MS}(2GeV)]^{1/3} = 263(3)(4)$ MeV and $F = 85.8(7)(20)$ MeV if F_K is used to set the scale by supplementing the theory with a quenched strange quark.



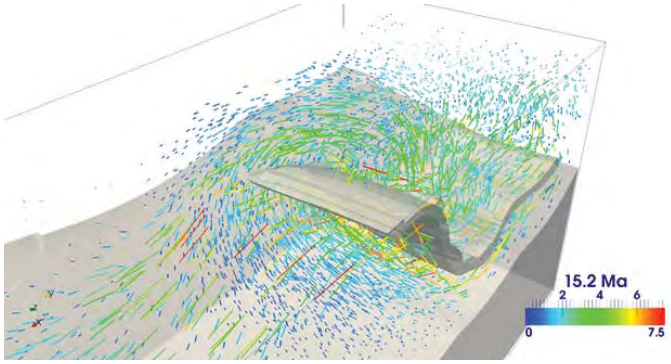
The pion mass squared versus the RGI quark mass, both normalised to $4\pi F$ which is roughly 1 GeV. The ratio $(M_\pi^2/2mF)^{1/3}$ is extrapolated to the continuum as in Eq. (6). The (central) solid line is the GMOR contribution to the pion mass squared computed by taking the direct measure of the condensate from the spectral density. The upper and lower solid lines indicate the statistical error band, while the dotted- dashed ones the total error.

ISCRA

Mid mantle seismic anisotropy around subduction zones

Manuele Faccenda
Padova University

There is increasing evidence for mid mantle seismic anisotropy around subduction zones whose interpretation remains elusive. In this study I estimate the strain-induced mid mantle fabric and associated seismic anisotropy developing in 3D petrological-thermo-mechanical subduction models where the slab is either stagnating over the 660 km discontinuity or penetrating into the lower mantle. The modelling of lattice-preferred-orientation (LPO) development of wadsleyite and perovskite has been calibrated with results from deformational experiments and ab-initio atomic scale models, and the single crystal elastic tensor of the different mineral phases is scaled by local P–T conditions. The lower transition zone (ringwoodite + garnet) is assumed to be isotropic. Mid mantle fabric develops in proximity of the subducting slab where deformation and stresses are high. The upper transition zone (wadsleyite + garnet) is characterized by weak transverse isotropy (2–3%) with symmetry axes oriented and fast S wave polarized dip-normal. A slightly stronger transverse isotropy develops in the lower mantle (perovskite + periclase), where the polarization of the fast S wave and the maximum Vp and dVs are parallel to the slab dip and subduction direction. These results may help in reconciling the seismic anisotropy patterns observed in some subduction zones with subduction-induced deformation, such as those measured in the mid mantle between the Australian plate and the New Hebrides–Tonga-Kermadec trenches that I interpret as related to stagnating portions of the subducted Pacific plate.



3D petrological-thermo-mechanical model of dynamic subduction. View from the mid-plane of symmetry. The subducting plate stagnates in the transition zone owing to the positive buoyancy arising from phase transition at the 660 km discontinuity. The white surfaces envelope material whose viscosity is greater than 9e+22 Pa s. The directions of maximum stretching in the mantle are indicated by the axes, whose color and length is scaled according to the amount of deformation.

Development of the atmospheric model CRAMS (Calabria Regional Atmospheric Modeling System)

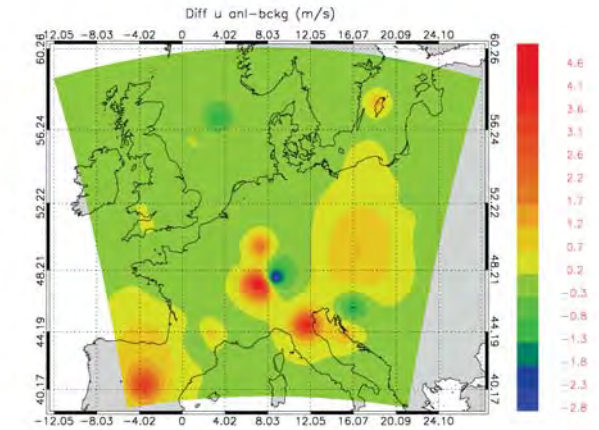
Stefano Federico
ISAC-CNR

The aim of the project is to develop a three-dimensional variational data assimilation system. The system can be used with different numerical weather prediction models, but it is mainly designed to be coupled with the Regional Atmospheric Modelling System (RAMS). Analyses are given for the following parameters: zonal and meridional wind components, temperature, relative humidity, and geopotential height.

Important features of the data assimilation system are the use of incremental formulation of the cost-function, and the representation of the background error by recursive filters and the eigenmodes of the vertical component of the background error covariance matrix. This matrix is estimated by the National Meteorological Center (NMC) method.

The data assimilation and forecasting system was applied to the real context of atmospheric profiling data assimilation, and in particular to the short-term wind prediction. The analyses were produced at 20 km horizontal resolution over central Europe and extended over the whole troposphere. Assimilated data are vertical soundings of wind, temperature, and relative humidity from radiosondes, and wind measurements of the European wind profiler network.

Results show the validity of the analyses because they are closer to the observations (lower RMSE) compared to the background (higher RMSE), and the differences of the RMSEs are in agreement with the data assimilation settings.



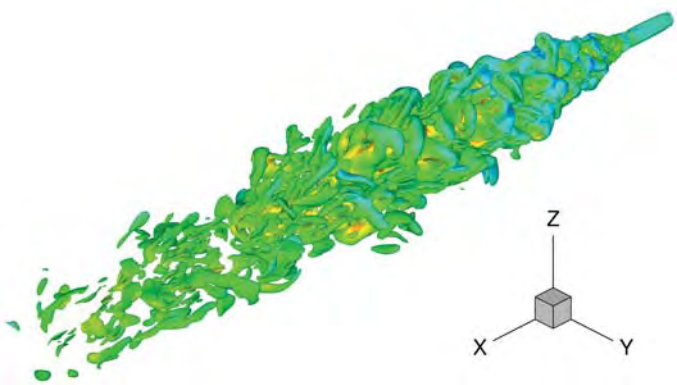
Analysis increments (m/s) of the zonal wind component (m/s) at 850 hPa at 12 UTC on 01 July 2012. The positions of the radiosoundings (open squares) and of the wind profilers (filled circles) used in the analysis are shown.

ISCRA

Large Eddy Simulation of High-Density Ratio Jets

Vinicio Magi
Basilicata University

The aim of this project is the analysis of hydrogen jets by using a Large Eddy Simulation model in order to gain new insights into the fluid dynamic process of turbulent mixing. The investigation of such jets is a relevant subject for the development of new propulsion systems, to improve the performance and the efficiency of direct-injection engines and also for safety issues. The computations of hydrogen jets require accurate and robust computational tools. Hence, the use of a suitable code and high performance computing is mandatory to successfully carry out the simulations.
The present work is carried out by means of an in-house code, named FLEDS. A significant issue when dealing with compressible free jets, especially with hydrogen jets, is the presence of sharp density gradients in the flow field, that cause non-physical spurious oscillations. In order to avoid these instabilities, an innovative localized Artificial Diffusivity Scheme has been implemented. The flow model has been assessed by comparing the numerical results with both theoretical considerations and experimental measurements.
The influence of both high air/hydrogen density ratios and jet Mach numbers on the turbulent mixing and the spreading rate has been analyzed by means of FLEDS code. This is a major issue dealing with direct injection in combustion systems, since the efficiency of combustion and pollutant emissions are strictly related to the mixing of air and fuel in diffusive flames.

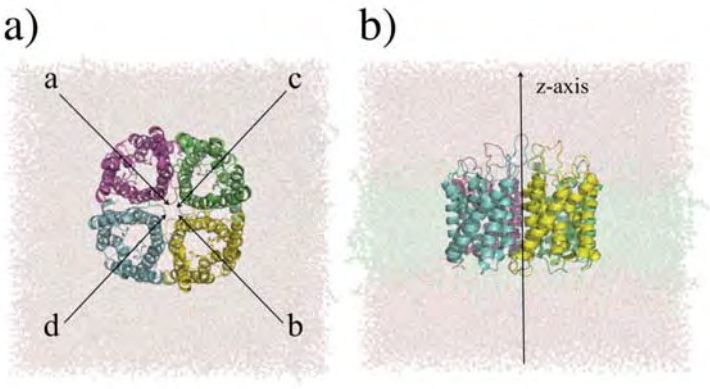


Large Eddy Simulation of a hydrogen jet: vorticity iso-surface coloured with Mach number values.
Bonelli F., Viggiano A., Magi V. (2013). AIP Conference Proceedings. vol. 1558, p. 232-235, http://dx.doi.org/10.1063/1.4825463

Epitope for Neuromyelitis Optica autoantibody binding in human aquaporin 4: exploring the role of highly conserved TM2 residues (acronym: epi-NMO)

Giuseppe Felice Mangiatordi
'Aldo Moro' Bari University

Neuromyelitis Optica (NMO) is a multiple sclerosis-like immunopathology disease affecting optic nerves and spinal cord. Its pathological hallmark is the deposition of a typical immunoglobulin, called NMO-IgG, against the perivascular water channel Aquaporin-4 (AQP4). This protein is able to form tetramers in the plasma membrane, which can further aggregate into supramolecular structures, called Orthogonal Arrays of Particles (OAPs). The prevention of the binding of NMO-IgG would represent a valuable molecular strategy for a focused NMO therapy. In this respect, the recent observation that Aspartate in position 69 (D69) is determinant for the formation of NMO-IgG epitopes [1] prompted us to carry out intensive Molecular Dynamics (MD) studies on a number of single-point AQP4 tetramer mutants. A domino effect was observed upstream. In particular, side chain of T62 was reoriented far from its expected position leaning on the lumen of the pore. More importantly, the strength of H-bond interaction between L53 and T56, at the basis of the loop A, was substantially weakened. Taken together, these events represent important pieces of the clear-cut mechanistic rationale behind the failure of the NMO-IgG binding, while the water channel function as well as the propensity to aggregate into OAPs remains unaltered.



a) Top view and b) lateral view of the investigated system. Water molecules and the membrane bilayer are rendered as sticks while the AQP4 tetramer is shown in cartoon representation.

[1] Pisani, F.; Mola, M. G.; Simone, L.; Rosito, S.; Alberga, D.; Mangiatordi, G. F.; Lattanzi, G.; Nicolotti, O.; Frigeri, A.; Svelto, M.; Nicchia, G. P. Identification of a Point Mutation Impairing the Binding between Aquaporin-4 and the Neuromyelitis Optica Autoantibodies. J. Biol. Chem. 2014

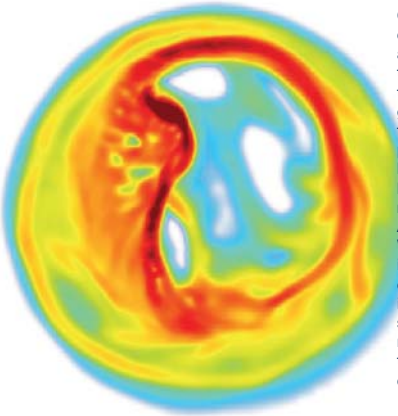
ISCRA

The fate of ring galaxies

Michela Mapelli
INAF

Ring galaxies, characterized by a bright ring of gas and young stars, are one of the most fascinating classes of galaxies in the Universe. According to the most popular scenario, these rings are the result of a dramatic galaxy-galaxy collision. If a bullet galaxy collides with a disc galaxy, the collision triggers a density wave propagating through the disc, similar to the rings produced by a pebble falling into a pond. Ring galaxies are one of the best laboratories to investigate the effects of strong galaxy interactions, and to understand star formation. Our aim is to shed light on two of the most pressing open questions about ring galaxies: [1] which is the impact of the interaction geometry on the properties of the ring? [2] which is the fate of old ring galaxies?

We performed N-body/Adaptive Mesh Refinement simulations of galaxy-galaxy collisions, using the public code RAMSES [3]. The figure shows the density map of gas in one of our simulations. We find that axisymmetric encounters produce circular primary rings followed by smaller secondary rings, while off-centre interactions produce asymmetric rings with displaced nuclei. The star formation history of our models is mainly influenced by the impact parameter: axisymmetric collisions induce impulsive short-lived starburst episodes (Fiacconi et al. 2012). We find that old ring galaxies might evolve into giant low-surface brightness galaxies, confirming the predictions by Mapelli et al. (2008).



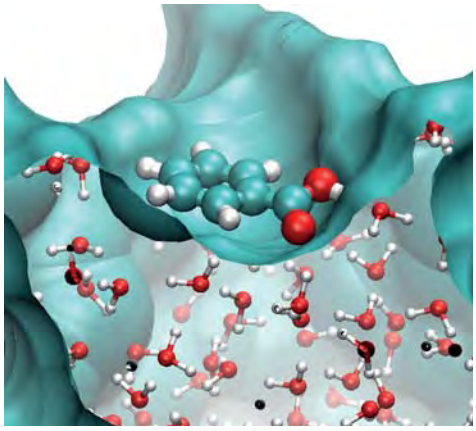
Collisional ring galaxies are characterized by a luminous ring of stars and gas. They are expected to form from the collision of a disc galaxy (hereafter the target galaxy) and a companion galaxy (hereafter the bullet galaxy). In the frame of the ISCRA HP10B3BJEW project, we simulated the collision between the target and the bullet galaxy by using the RAMSES adaptive mesh refinement code (Teyssier 2002, Astronomy & Astrophysics, 385, 337). We ran a large set of simulations, investigating the importance of different collision parameters (impact parameter, inclination and relative velocity). The plot shows the mass-weighted gas density map in the xy plane (i.e. the plane of the target disc) at time = 50 Myr after the collision for one of our simulations.

[1] Fiacconi D., Mapelli M., Ripamonti E., Colpi M., Adaptive mesh refinement simulations of collisional ring galaxies: effects of the interaction geometry, 2012, MNRAS, 425, 2255
[2] Mapelli M., Moore B., Ripamonti E., Mayer L., Colpi M., Giordano L., Are ring galaxies the ancestors of giant low surface brightness galaxies?, 2008, MNRAS, 383, 1223
[3] Teyssier R., Cosmological hydrodynamics with adaptive mesh refinement. A new high resolution code called RAMSES, 2002, A&A, 385, 337

Acid Dissociation at aiR/wAter InterfaCe

Marco Masia
Sassari University

Carboxylic acids are important and ubiquitous in chemistry, biology, as well as heavy crude oils. Acidity of an acid depends on not only its chemical structure, but also its solvation condition. Acidity rankings sometimes reverse in different media: acetic acid is more acidic than propionic acid in aqueous solutions; but the opposite is true in the gas phase. Acidities in those bulk media have been well studied both experimentally and theoretically; however, they are poorly understood on surfaces and interfaces where acids are partially solvated. In this project, that pertains to a wider theoretical/experimental collaboration, we have investigated the mechanism for dissociation of weak organic acids at the water/air interface by means of first principle Molecular Dynamics (MD) simulations. In particular we studied the potential of mean force (free energy) for dissociation of acetic and benzoic acid at water surface. In addition, the influence of the solvation patterns on the activation barrier for the proton transfer has been addressed; using constrained MD simulations we characterized the restructuring of the hydrogen bond network upon acid dissociation. To our best knowledge there are not previous theoretical studies of organic acid dissociation at the air/water interface. Therefore, we believe that this study will establish a reference to answer fundamental questions of structure-interfacial property relationship and how different hydration structures influence thermodynamics of reactions on surfaces.



Snapshot from the Molecular Dynamics simulation showing a molecule of benzoic acid lying at the interface between water and air before proton dissociation.

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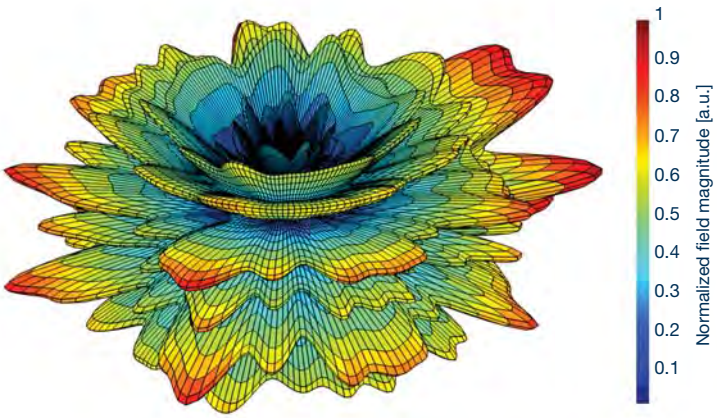
Numerical Investigation into the Performance of Plasma Antenna Array

Davide Melazzi
Padova University

Gaseous Plasma Antennas (GPAs) are devices that rely on a partially or fully ionized gas (rather than just metallic parts) to radiate electromagnetic waves. That is why GPAs have potential advantages over conventional metallic antennas: (i) GPAs are reconfigurable with respect to input impedance, radiation pattern, frequency of operation and bandwidth; (ii) they can be reconfigured electrically - rather than mechanically - on time scales the order of microseconds to milliseconds; (iii) they are virtually "transparent" above the plasma frequency and become "invisible" once turned off. Last but not least, GPAs operating at different frequencies do not interfere with each other - which enables stacking arrays of antennas. A group of GPAs and, possibly, metallic antennas is called a plasma antenna array (PAA).
Experimental investigation into the performance of GPAs and PAAs have been supported mostly by simplified numerical approaches. To assess the role of the plasma discharge parameters in the radiation efficiency of a plasma antenna, we use ADAMANT (Advanced coDe for Anisotropic Media and ANTennas), which features a full-wave approach based on the numerical solution of coupled surface and volume integral equations.
In this work we report on the analysis of a reconfigurable PAA comprised of a metallic half-wavelength dipole that is surrounded by cylindrical plasma tubes arranged in a planar circular lattice, that exhibits reconfigurable beam-forming and beam-steering capabilities.

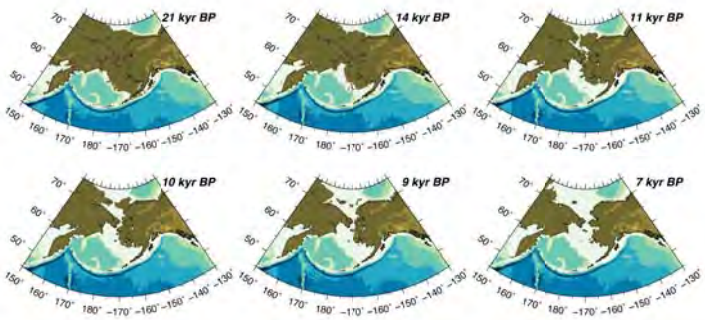


Far field radiation pattern of a plasma antenna array references: D.Melazzi,V.Lancellotti, "ADAMANT: a surface and volume integral-equation solver for the analysis and design of helicon plasma sources", Comp. Physics Comm., vol 185, no. 7, July 2014, pp.1914-1925

Modeling postglacial sea-level change with SELEN

Daniele Melini
INGV

In the framework of global change, understanding the contribution of the melting of continental ice sheets to future sea-level rise is one of the major scientific challenges. The physical processes governing the glacio-hydro-isostatic sea-level changes have been thoroughly studied in the last decades; they are quantitatively described by an integral equation called "Sea Level Equation" (SLE), which relates sea-level variations to the evolution of ice sheets volume and to the rheology of the Earth's mantle. Past, present and future variations of sea-level in response to ice sheet melting can be modeled by solving numerically the SLE. It accounts for both the short-term elastic response of the Earth and for the long-term visco-elastic deformation, also taking into account the gravitational attraction between the solid Earth, the oceans and the ice sheets. The SLE can be adapted to account also for shoreline migration, whose effect is particularly important in key areas such as the Mediterranean Sea and represents a crucial factor in the assessment of coastal hazard in consequence to sea-level rise. A numerical solution of the SLE, suitable for the modelling of the regional and the global sea-level variations associated with fluctuations of the continental ice sheets, can be obtained numerically with the SELEN code, the only open source SLE solver, available through the Computational Infrastructure for Geodynamics (CIG) website (http://www.geodynamics.org).



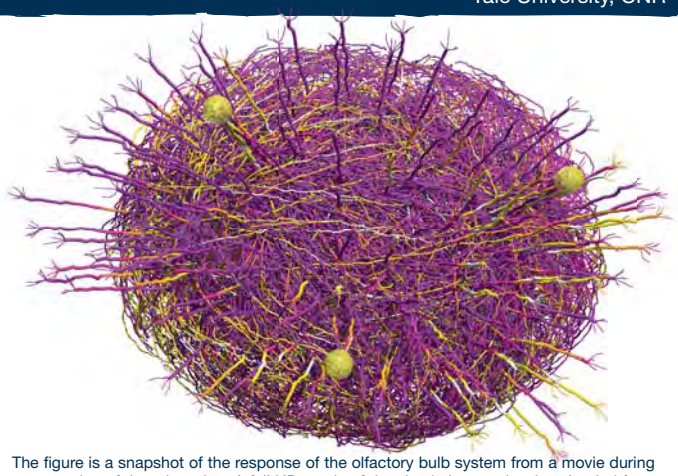
Shoreline migration and sealevel change in the Beringia region at since the Last Glacial Maximum (21kyrs before present). The maps are the result of an high-resolution solution of the "Sea-Level Equation" assuming the ICE-5G deglaciation model (Peltier, 2004). Paleo-topography evolution in Beringia is particularly important in view of its impact on migrations between North America and Asia. Numerical computations have been performed on the FERMI system at Cineca with the SELEN code (http://www.geodynamics.org).

ISCRA

3DBULB

Michele Migliore
Yale University, CNR

A clear understanding of the spatio-temporal dynamics of olfactory bulb mitral cells in representing an odor input is very difficult to achieve experimentally; for this reason, the activity-dependent effects of olfactory bulb network self-organization generated by the mitral-granule cell microcircuits remain poorly understood. To deal with this problem, we have constructed olfactory bulb microcircuits using realistic three dimensional (3D) inputs, cell morphologies, and network connectivity.
The computational approach is based on a novel NEURON + Python fully integrated parallel simulation environment, that can be applied to other regions as well. A population of approximately 700 synthetic mitral cells and 120,000 granule cells were randomly connected using a collision detection algorithm. Intrinsic optical imaging data obtained during presentation of 19 natural odors was used to drive self-organization of the network under different conditions of odor inputs.
The results provided new insights into the relations between the functional properties of individual cells and the network in which they are embedded, making experimentally testable predictions on odor processing and learning.

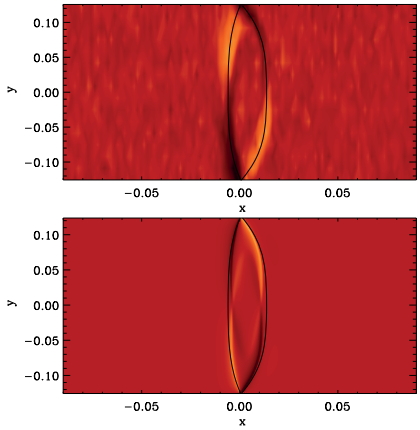


The figure is a snapshot of the response of the olfactory bulb system from a movie during presentation of the mint odor. A full HD movie of the simulation can be downloaded from the the ModelDB section of the Senselab database suite (http://senselab.med.yale.edu, acc.n. 151681).

MARCEL3D

Anna Perona
Pisa University

The purpose of the MARCEL3D project was to perform an extensive benchmark of a three-dimensional (3D) test-particle code for the investigation of the electron behaviour in the region where a magnetic reconnection process occurs. Such a tool (whose writing had been carried out during the previous ELKREC3D B-project) is based on a 3D cartesian relativistic model of the electron guiding-center dynamics in the presence of the fields characterizing a non-steady-state MHD description of magnetic reconnection. The test-particle code is able to follow the dynamics of single particles and the global response of an electron population during the evolution of the reconnection fields, thus allowing the calculation of the electron kinetic moments at different stages of the process in quite realistic reconnection configurations.
In particular, we have tested the performances of this electron code by coupling it to a fluid collisionless reconnection code where a strong guide field is present and where the change in the magnetic topology is driven by the electron inertial term in the generalized Ohm's law.
This work represents a first step towards a fully self-consistent reconstruction of the process, where the kinetic results will be fed back to the fluid description. Already at this first stage, however, such a test-particle method allows for an easier understanding of the role played on the electron behavior by the physical terms included in different fluid reconnection models. Results have been described in Computer Physics Communications, 185 (1), pp. 86, 2014.



Comparison between the contour levels of the kinetic electron density (left) and of the fluid vorticity (right) during the nonlinear phase (294 τA). The black line represents the separatrix of the magnetic island calculated by the fluid reconnection code.

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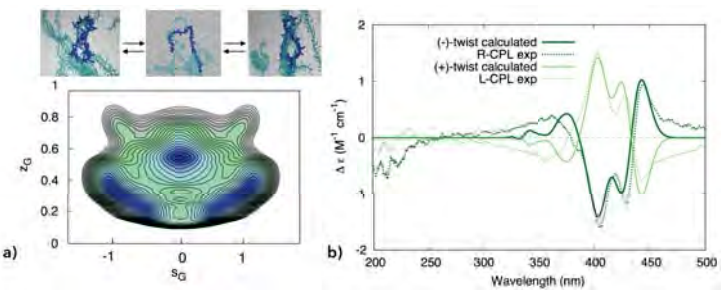
Predicting the chiral harvesting through free-energy methods

Adriana Pietropaolo
Catanzaro University

Artificial polymers can exhibit a switchable screw-sense whose inversion is conducted by chemical or photo stimuli [1-2]. Within the PRACE framework, we worked on the reconstruction of the free energy landscape of a class of optically inactive polyfluorene-based polymers, the poly (9,9-dioctylfluoren-2,7-diyl) (PDOF), whose single-handed circularly polarized light (CPL) selectively induces a chiral harvesting [3]. The free energy landscape reconstructed for sixteen chains of PDOF deposited on amorphous silica afforded two enantiomeric free energy basins, with all-negative and all-positive twist dihedrals and one racemic free energy basin. In order to validate the former free-energy landscape, we calculated owing to ISCRA resources the ECD spectra in the TD-DFT framework for the 2,2'-difluorenyl using the B97-D functional, that includes damped atom-pairwise dispersion corrections [4]. We then proceeded to calculate the ECD spectra through the ZINDO method [5,6] on PDOF decamer sections corresponding to the two enantiomeric free-energy basins. Those coordinates show rotational strengths affording ECD spectra strikingly similar to CD spectra experimentally recorded.

[1] Nakano , Okamoto, Chem. Rev. 2001, 101, 4013
[2] Pietropaolo, Nakano. J. Am. Chem. Soc. 2013, 135, 5509
[3] Wang, Sakamoto, Nakano, Chem. Commun. 2012, 48, 1871
[4] Grimme. J Comput Chem. 2006, 27, 1787
[5] Ridley, Zerner. Theor. Chim. Acta 1973, 32, 111
[6] Ridley, Zerner, J. Mol. Spectrosc. 1974, 50, 457



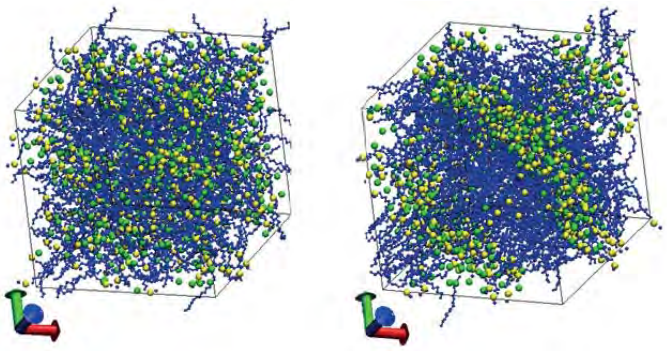
a) The PDOF free energy landscape.
b) ECD spectra calculated for the enantiomeric basins. Experimental spectra are also reported for comparison.

Coarse-Grained MD simulations of Ionic Liquid Crystals

Giacomo Saielli
CNR, Padova University

We have investigated the mesomorphic properties of a model Coarse-Grained Force Field initially developed for the isotropic phase of short chain imidazolium salts [1]. MD simulations, using the software DL_POLY on the CINECA's Super Computer FERMI, allowed to explore the phase diagram of the system [C16mim][NO3] and to identify the range of existence of a SmA phase. Thus, the model potential has been employed to investigate the structural and dynamical properties of this model of imidazolium-based Ionic Liquid Crystals (ILCs). In a first paper we have studied the structural properties of ILCs, that is the translational and orientational order of the liquid crystal phase [2]; in a second paper we have investigated the dynamic properties, in particular the ratio between the parallel and perpendicular diffusion coefficients, and the mechanism of diffusion [3]; finally we have analyzed the isotropic-to-smectic A transition using the heterogeneity order parameter (HOP), which is a direct measure of the degree of microsegregation between charged parts and hydrophobic alkyl chains [4].

[1] Y. Wang, S. Feng, G. Voth, J. Chem. Theory Comput. 2009, 5, 1091-1098
[2] G. Saielli, Soft Matter 2012, 8, 10279-10278. Hot Paper: http://blogs.rsc.org/sm/2012/12/13/
[3] G. Saielli, G. A. Voth, Y. Wang, Soft Matter 2013, 9, 5716-5725
[4] G. Saielli, A. Bagno, Y. Wang, manuscript in preparation



The two snapshots show the transition from the isotropic (left) to the SmA (right) liquid crystal phase of the Coarse-Grained model system of [C16mim][NO3] on cooling. Yellow: imidazolium cation's head; green: anion; blue: alkyl chain. Graphic rendering with VMD (www.ks.uiuc.edu/Research/vmd/)

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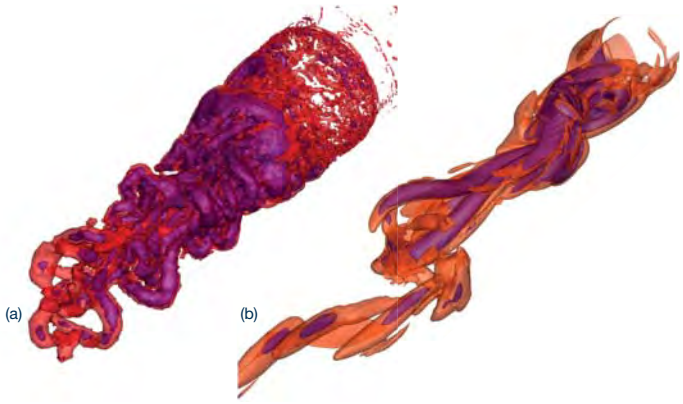
Bluff-Body Base Drag REDuction through boundary-layer modification B3DRED

Maria Vittoria Salvetti
Pisa University

The main contribution to the aerodynamic drag of a bluff body is normally given by the low pressures acting on its base, which is the part of the body surface lying within the separated wake. Decreasing the base drag
would then have a considerable importance in many engineering applications, such as the design of low-consumption road vehicles. Thus, a preliminary critical issue with significant scientific interest is the characterization of the relationship between the base pressure and the parameters defining a particular flow configuration, and, especially, the identification of the physical origin of this relationship.
The variation of the base drag of an axisymmetric bluff body caused by modifications of the boundary-layer separating at the sharp-edged contour of its base is analyzed through different numerical simulations, and the results are compared with those of a previous experimental investigation. Variational MultiScale Large-Eddy Simulations (VMS-LES) are carried out on the same nominal geometry and at the same Reynolds number of the experiments. Direct Numerical Simulations (DNS) are also performed at Reynolds numbers that are roughly two orders of magnitude lower, in order to investigate on the sensitivity of the main findings to the Reynolds number. The results of experiments, VMS-LES and DNS simulations show that an increase of the base pressure – and thus a decrease of the base drag – may be obtained by increasing the boundary layer thickness before separation, which causes a proportional increase of the length of the mean recirculation region.

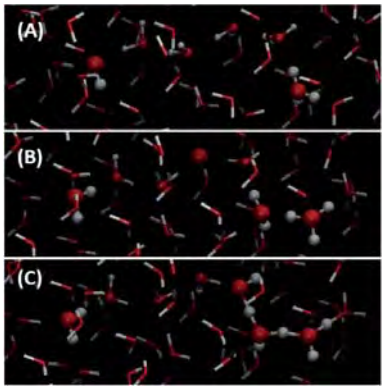


Hairpin vortices characterizing the dynamics of the near wake: VMS-LES (a) and DNS (b).

Ionic recombination mechanisms in ice

Sandro Scandolo
ICTP

One of the most fundamental processes in acid-base chemistry is the ionization of water resulting in the formation of water's constituent ions, the hydronium and hydroxide. In the liquid phase, these chemical processes involves a complex interplay of collective vibrations, rotations and the reorganization of hydrogen bonded networks and hence the coupling of many different degrees of freedom. In our ongoing project at Cineca, we have been looking at the molecular mechanisms associated with the recombination of hydronium and hydroxide ions in solid---water Ice-Ih. We employ state of the art ab initio molecular dynamics simulations with cells made up of 288 water molecules. In these calculations, the electronic degrees of freedom are explicitly treated. Figs A-C illustrate some of the essential steps of the recombination process that are emerging from our ongoing calculations. What is quite interesting here in contrast to liquid water is that the hydroxide ion appears to be more labile compared to the proton in the recombination process. Furthermore, both the ion hopping events involve highly concerted proton motions. We are now exploring how defects, such as vacancies and interstitials in close vicinity of the ions alter the underlying mechanisms.



(A) At time t=0, the ions are separated from each other by a water wire consisting of 5 hydrogen bonds.
(B) Within less than 300 fs, the hydroxide ion quickly shuttles across three hydrogen bonds getting closer to the hydronium.
(C) In the next 100 fs, both the hydronium and hydroxide then find each other and undergo neutralization.

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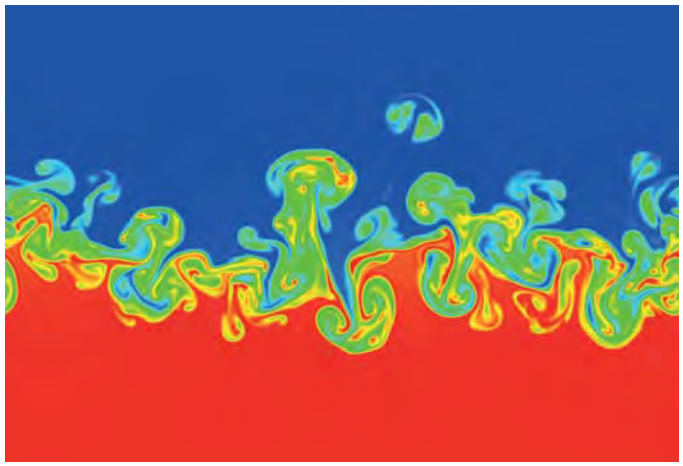
Simulation of the Rayleigh-Taylor Instability

Sebastiano Fabio Schifano
INFN

The Rayleigh-Taylor instability arises every time a higher density fluid is stacked over a less dense one in the presence of gravity. At the contact surface an instability is triggered that mixes the two till the equilibrium is reached. This can be a familiar phenomenon, happening for instance if cold wine is gently poured in a glass half-filled with warmer water.
However the Rayleigh-Taylor instability is relevant in many areas of science and technology, ranging from thermal engineering to astrophysics, and its theoretical understanding is far from being complete. Numerical simulations are a key tool to investigate this phenomenon.
The picture illustrates the dynamics of a Rayleigh-Taylor unstable fluid, simulated on a parallel computer with the Lattice-Boltzmann technique, using a discretized cell of size 1024x2048 grid-points.
The snapshot shows a temperature map (blue coldest, red warmest temperature) of the time evolution of the sistem. One sees clearly the development of tipical "plumes" that emerge from the cotact interface of the two fluids in an orderly way and quick develop a cahotic behaviour.
This dynamics mixes the warm and cold parts of the fluids till eventually an equilibrium is reached.
This visualization uses data of a science project performed by a collaboration of INFN and the Universities of Ferrara, Roma Tor Vergata, and Eindhoven.



Temperature map at an early stage in the evolution of the Rayleigh-Taylor instability.

Orientation and behavior of the oxonine dye in the one-dimensional nanochannels of zeolite L.

Gloria Tabacchi
Insubria University

This work solves a long-standing problem on an important class of optical nanomaterials, provides the knowledge bases for improving their functionality and uncovers a novel, surprising type of molecular motion: squid-like diffusion.
Hybrid materials with outstanding optical properties can be fabricated by using organizing hosts with channel diameters in the order of one nanometer, such as zeolite L. Its one-dimensional (1D) channels can act as ordering nanocontainers for photoactive species, leading to applications in key technological areas, such as solar energy harvesting, information processing and bionanomedicine. Orientation of the encapsulated dye molecules greatly influences the functionality of the resulting host-guest material. The orientation of the dye oxonine has been an enigma since the early days of dye-zeolite L technology. Fluorescence microscopy experiments suggest that the oxonine molecular axis forms a 70° angle with the zeolite channel axis, but such orientation is incompatible with the relative dimensions of molecule and channels. Now, computer simulations of the Oxonine-zeolite L material unravel the orientation of oxonine, reveal that it is determined by water and explain the observed optical properties on the basis of the molecular-level behavior of the dye. The oxonine squidlike motion sketched in the movie suggests that molecular flexibility may play a key role in switching the dye orientation.

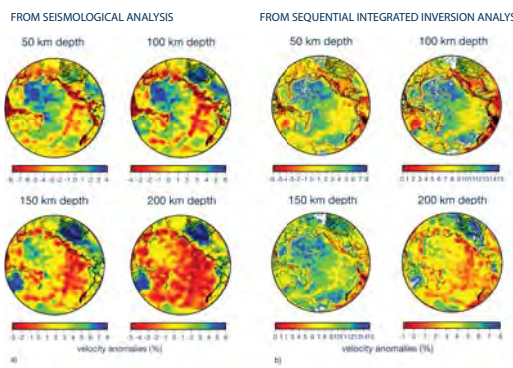
Diffusion mechanism of a dye molecule (oxonine) along the nanochannels of zeolite L.
Left: the molecule is oriented perpendicular to the channel axis; with this orientation, the molecule is trapped in one cage and cannot diffuse along the channel. Right: the molecule is oriented parallel to the channel axis; with this orientation, the molecule can move from cage to cage.
Middle: the transition from the perpendicular to the parallel orientation is achieved by a squid-like bending of the dye molecule.
E. Fois, G. Tabacchi, G. Calzaferri Orientation and Order of Xanthene Dyes in the One-Dimensional Channels of Zeolite L: Bridging the Gap between Experimental Data and Molecular Behavior , J. Phys. Chem. C 2012, 116, 16784–16799.

ISCRA

Optimization of dense matrix applied to the analysis of Pacific Ocean geophysical data sets

Maria Rosaria Tondi
INGV

With this project, we have tested the feasibility of the computational problem related to the joint optimization of seismological and gravity data acquired in the area of the Pacific region (90°S 90°N) (121°E 60W). In order to reach our goals we have decided to adopt the algorithm of Sequential Integrated Inversion (SII). It is a fast and effective way to integrate the information given by seismological and gravity datasets, which deals with the presence of irreducible dense matrices (Tondi et al., 2012).
Our model is discretized on a 1° x 1° regular grid and a depth of 350 km, for a 544,680 parameters to be optimized.
The seismic information is recovered from the surface waveform tomography of the Pacific upper mantle, obtained at the Université Louis Pasteur in Strasbourg (Maggi et al., 2006) (Fig. 1 (a)). Hence, the velocity model has been iteratively updated and scaled to a 3-D density model through the SII inversion approach.
We considered a set of 514,085 gravity observations extracted from the gravity models from the ESA Earth's explorer GOCE (Gravity field and Ocean Circulation Explorer) mission (Drinkwater et al. 2003). As a result, the FERMI system, which has been used to handle computations, had to deal with a dense matrix sized 544,680 x 514,085 (memory to be allocated: 2086.25 Gb).
The results (Fig. 1 (b)), show an improved crustal and upper mantle earth model of the Pacific region, a topic area for the understanding of the structure and evolution of oceanic plates.



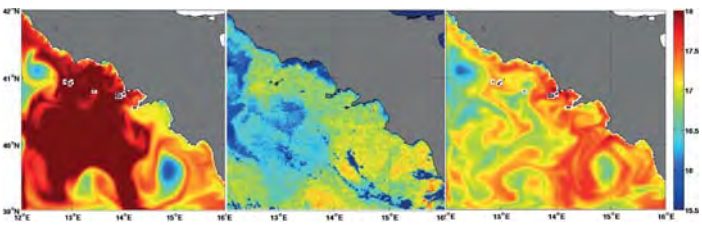
a) Depth sections of the shear velocity percentage perturbations in the 3D model of the Pacific region, obtained with the analysis of the seismological data-set. b) Depth sections of the shear velocity percentage perturbations in the 3D model of the Pacific region, obtained with the analysis of both the seismological data-set and the gravity data-set through the parallel procedure of Sequential Integrated Inversion.

Drinkwater, M.R., Floberghagen, R., Haagmans, R., Muzi, D. and Popescu, A., 2003. GOCE: ESA's first Explorer Core mission. Space Science Reviews, 108, 419-432.
Maggi, A., Debayle, E., Priestley K., and Barruol, G., 2006. Multimode surface waveform tomography of the Pacific Ocean: a closer look at the lithospheric cooling signature. Geophys. J. Int., 166, 1384–1397, doi: 10.1111/j.1365-246X.2006.03037.x.
R. Tondi, C. Cavazzoni, P. Danecek, A. Morelli, 2012. Parallel, 'large' dense matrix problems: Application to 3D sequential integrated inversion of seismological and gravity data, Computers and Geosciences, 48, 143-156.

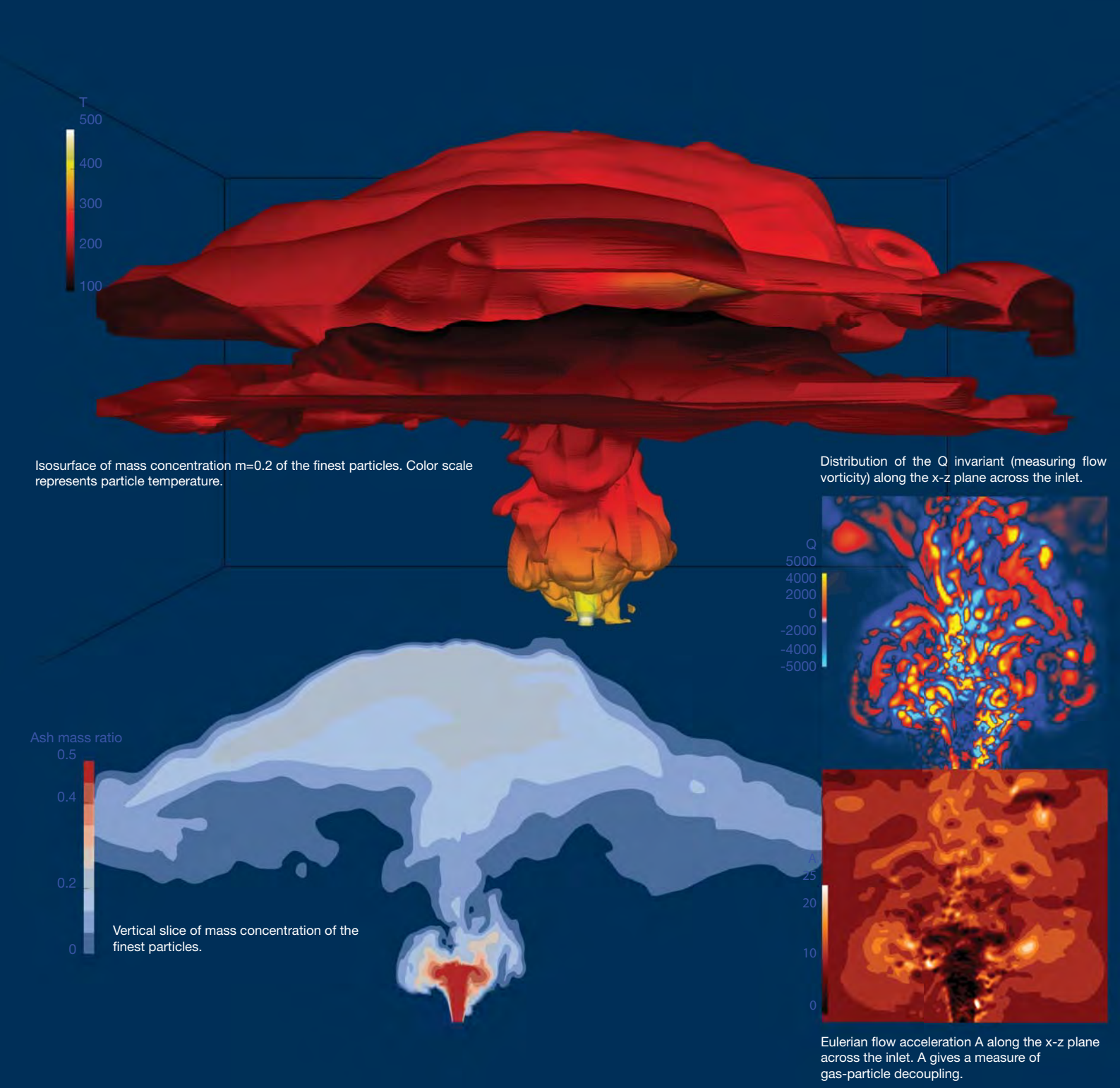
Nested nUmerical Models to Investigate Submesoscale COastal processes (NUMISCO)

Enrico Zambianchi
Parthenope Naples University, CoNISMa

NUMISCO project was an important step towards a better understanding of coastal dynamics through high spatial and temporal resolution numerical simulations. The main scientific objective was to simulate the 3-D circulation in the Gulf of Naples (GoN) dominated by buoyancy input and wind forcing, influenced by complex bathymetry and interacting with the open ocean, and to determine how the circulation patterns control the transport of waterborne materials (particularly pollutants) through these regions. We applied an advanced "four dimensional variational method (4D-Var)" of data assimilation (DA) to a sophisticated coastal numerical model (the Regional Ocean Modeling System, ROMS) configured at medium resolution (3km) and nested into the Mercator-Ocean High Resolution ocean forecasting system in the Atlantic and Mediterranean basins.
Different types of data were utilised: satellite sea surface temperatures (SST) and real-time surface velocity data provided by a system of high frequency (HF) coastal radars, operating in the GoN since 2004 and providing real-time hourly surface current fields with a resolution of 1.0 x 1.0 km. 4D-Var approach was applied in the ROMS domain with the aim to assess the skill of the DA procedure and to gain the best representation and understanding of GoN coastal dynamics. The assimilation of HF radar data in coastal ocean models represents an innovative and novel approach within the Italian scientific community. The activity was supported by the National Flagship Project "RITMARE" (SP3-WP4-AZ6).



Comparison between the SST fields obtained by the ROMS model simulation before (left panel) and after (right panel) the application of the 4-dimensional data assimilation technique with respect to the AQUA-MODIS (1 km single swath) SST field in December 2009 (centre panel).



Three-dimensional numerical simulation of an eruption column in a stable atmosphere. Inflow parameters represent typical eruption conditions for a Plinian eruption (mass flow rate = 1.5 x 10^9 kg/s; exit velocity = 275 m/s; water content = 5 wt.%; temperature = 1053 K). Two particle classes of (d=0.5 mm; rho=2500 kg/m^3) and (d=15 microns; rho=2700 kg/m^3) are considered.
M. Cerminara, T. Esposti Ongaro “A fast Eulerian model for volcanic ash plumes”, 2014

LISA

MIRA: Numerical and experimental study for the prediction of the steady, three dimensional flow in a turbine nozzle vane cascade using OpenFOAM

The present study is the first step toward the application of the OpenFoam Toolbox to high pressure turbine modeling. The main goal is to exploit the joined perspectives of the High Performance Computing facilities available at Cineca and the license-free business model provided by OpenFoam. The object of the investigation is a solid vane (without film cooling) typical encountered in a high pressure turbine stage of a modern heavy-duty gas turbine engine, whose aerodynamic behavior has been characterized by EST Laboratory testing (Figure 1). In particular, the simulated vane profile is characterized by a pitch-to-chord ratio of s/c = 1.04 and an aspect ratio of H/c = 0.69, with a design flow turning of 70°. Uncompressible steady state RANS simulations were performed by using the *simpleFoam* solver. Two-equation turbulent models such as Standard k-ε, Realisable k-ε and the Shear Stress Transport (SST) k-ω were chosen to provide closure. In particular, the first model was used to carry out the mesh sensitivity analysis. The last two models, which are commonly used in industrial turbomachinery applications, were applied to the final mesh to seek the most accurate prediction of aerodynamic performance. CFD data were compared against the available experimental data base in order to perform a complete validation. The following aerodynamic measurements were considered:

- vane loading measured by means of instrumented vanes;
- midspan blade to blade flow measured by a 2D Laser Doppler Velocimetry system;
- total pressure distribution in wake region at midspan, at X/c_{ax} = 1.50;
- kinetic energy loss coefficient ζ distribution calculated from a 5-hole probe traversed along a plane at X/c_{ax} = 1.53

The most reliable turbulence model for wake predictions, i.e. SST k-ω, was further validated against experimental measurements of secondary flows, on a plane located at 53% cax downstream of the trailing edge, visualizing the kinetic energy loss coefficient ζ (Figure 2). With regard to measurements, most of the flow field is dominated by the passage vortex, as confirmed by the large, squeezed region of high losses on the suction side (SS) of the wake. The intensity and the extent of the passage vortex are related to aerodynamic load. In this case, the high pitch-to-chord ratio can be considered responsible for a quite intense passage vortex. The loss peak associated with the corner vortex is higher than the one generated by the passage vortex. It can be observed that the wake is relatively thick and the 2D region is confined to a narrow span around the midspan (from about Z/H = 0.3 to 0.7). From the comparison between experimental and numerical results, it emerged that the main vortical flow structures are correctly identified by SST k-ω turbulence model. However the kinetic energy losses associated with the passage vortex and the corner vortex are overestimated.

The preliminary outcomes of the analysis are therefore encouraging in terms of both accuracy with respect to experimental data and computational efficiency on HPC platforms.

Silvia Ravelli
Bergamo University

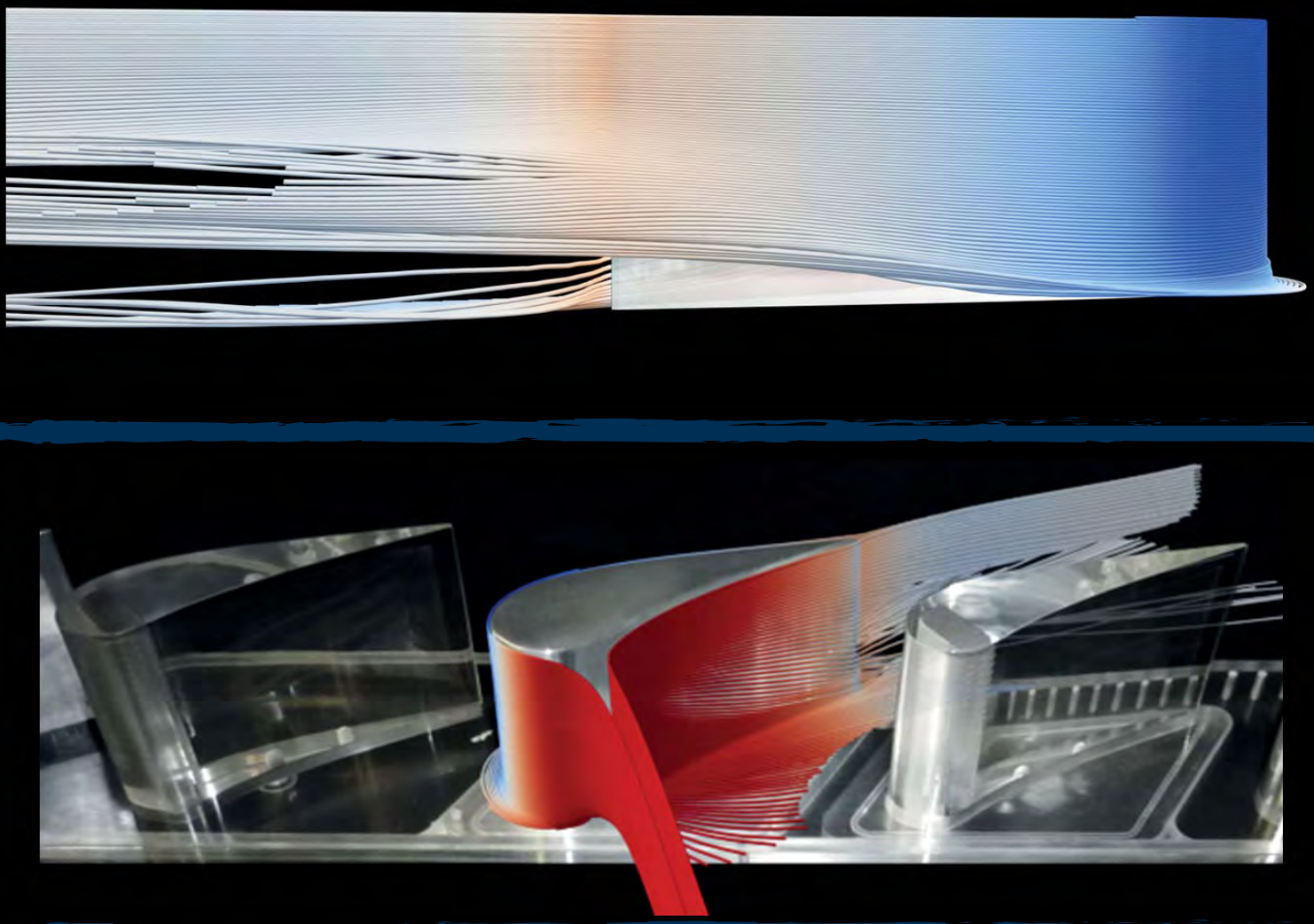
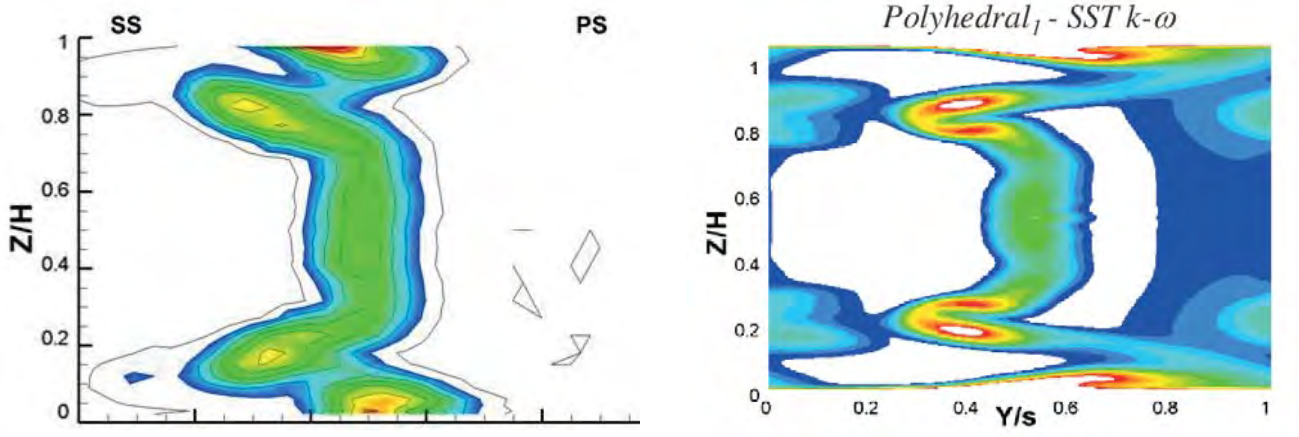


Figure 1: High loading profile of a modern heavy duty GT: experimental setup and visualization of computed flow structures colored by pressure distribution.

Figure 2: Experimental versus CFD modelling: Kinetic energy loss coefficient ζ distributions (X/c_{ax} = 1.53).

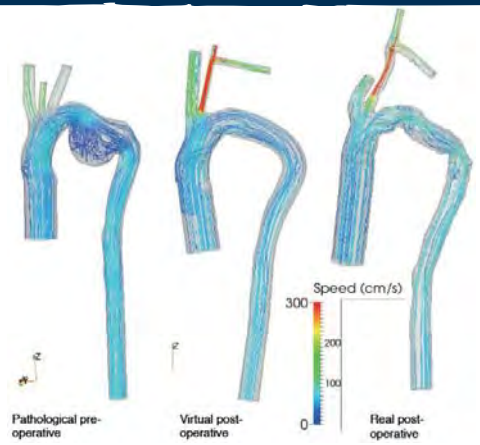


LISA

(PASCA2L) PAtient Specific Computational Analysis of Aortic hemodynamics over Large data sets

Ferdinando Auricchio
Pavia University

In 2014, we continued to work in collaboration with surgeons from Policlinico San Donato Hospital on Computational Fluid Dynamics (CFD) techniques for the study of aortic fluxes in physiological, pathological, and post-operative conditions.
We focused on performing full patient specific simulations on pre-, post-, and virtually postoperative geometries. We mean by virtually that we constructed, from a pathological pre-operative aortic shape, a geometry that mimics the aorta after surgery. With this procedure and the use of CFD techniques we provide a predictive tool to clinicians that they can use before surgery to observe, in-silico, possible surgical outcomes.
Preliminary results depicted in Figure clearly show that the simulation using a post-operative virtual geometry shares similar trends with the real post-operative situation. Further researches will focus on validation of the results, in particular with respect to magnetic resonance imaging techniques.

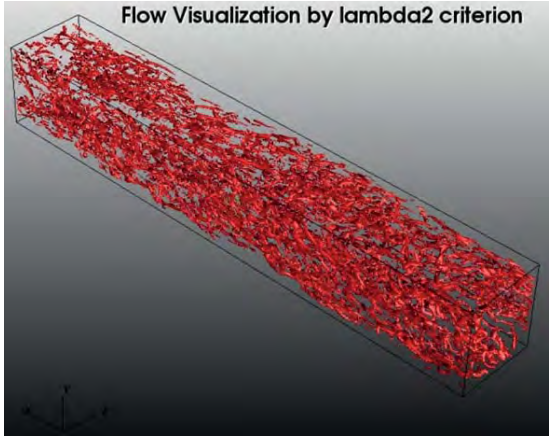


Patient with an aneurism which has been treated using a Thoracic Endovascular Repair (TEVAR) surgery. The figure shows streamlines, depicting speed. The numerical results show clear similarities between the virtual and real situations.

DNS4MODELING
DNS approach for industrial modeling development

Fabio Inzoli
PoliMI

The aim is to build a statistical fluid dynamics database for high Reynolds numbers with heat transfer to support the development and the assessment of LES/RANS turbulence models for complex fluid flow and heat transfer phenomena.
DNS approach is used to perform simulations, from which flow statistics are extracted to build the database. The Open Source Code Nek5000, developed at the Argonne National Laboratory and based on the spectral element method for unstructured hexahedral grids, has been used.
For this project, DNS computations are performed for the flow and heat transfer in two characteristic geometries, selected for their relevance in turbulence and heat transfer modeling, chosen as test cases: smooth and ribbed (90° ribs) straight square ducts (SD). For both geometries, the flow under investigation is characterized by a Reynolds number based on hydraulic diameter and bulk velocity equal to 10320.
The ribbed SD is characterized by a two-pass configuration (aligned ribs on the top and bottom walls), with a blockage ratio of about 30%. For both geometries, the flow is considered as fully developed and periodic boundary conditions are used in the stream-wise direction. For the ribbed SD, such periodic configuration includes only one rib (per wall).
For both analyzed geometries, statistics are collected for first order quantities, like mean pressure, temperature, stream-wise and secondary velocities, as well as higher order ones, like variances and co-variances. In Figure, an example of flow visualization, based on the lambda2 criterion, is reported for the SD.



Lambda2 criterion visualization for smooth Square Duct geometry

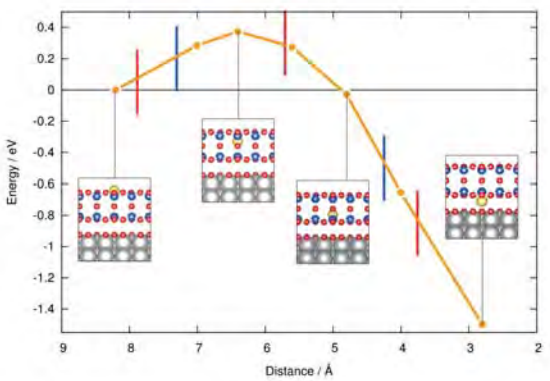
LISA

Nanostructured oxides: new materials for energy and environment

Adsorption of Li, Na, K and Mg Atoms on Amorphous and Crystalline Silica Bilayers on Ru(0001): A DFT Study

Gianfranco Pacchioni
Milano-Bicocca University

Oxide thin films are of great technological importance as insulating layers in integrated circuits or as supports for metal nanoparticles in sensors and catalysis. Ultra-thin oxide films exhibit special features, which emerge with decreasing film thickness. The surface structure can be modified in a controlled manner by the proper choice of the supporting material. The support can influence the growth direction of the oxide thin film and can interact with adsorbates, which are deposited on the thin film, and so influence their chemistry. Among crystalline ultra-thin films, silicon dioxide has been intensively investigated in the recent past. Silica mono- and bilayers are also denoted as silicatene, the silica analogs of graphene. Silica monolayers consist of SiO4 tetrahedra, which are bound together by 3 of 4 oxygen corners. Silica bilayers (double-layer silicatene) consist of two layers of SiO4 tetrahedra and bind to supporting materials by dispersion forces. We have studied the interaction of Li, Na, K and Mg atoms with crystalline and amorphous silica bilayers grown on Ru(0001) supports by performing DFT calculations. (Si4O6H4)n clusters have been chosen to represent different ring sizes (n=4-8) of amorphous silica bilayers. We found that on unsupported silica films the alkali metal atoms adsorb as neutral entities with weak adsorption energies, whereas the diffusion into the cage is not thermodynamically favorable. Interaction of Na with Al-doped silica cages has also been investigated. The presence of this Al-dopant enhances the strength of the metal-framework interaction changing completely the bonding mechanism which is dominated by charge transfer contributions. Na and Mg interacting with a crystalline silica bilayer on a 3O(2 × 2)/Ru(0001) surface adsorb preferentially at the interface between the support and the silica film with high adsorption energies and transfer their valence electrons to the Ru metal. The results show that the silica bilayer acts therefore as “inert” nanoporous membrane that allows a selective diffusion of atomic species to the surface of the metal support.



Interaction of Li, Na, K and Mg with supported and unsupported silica bilayers.

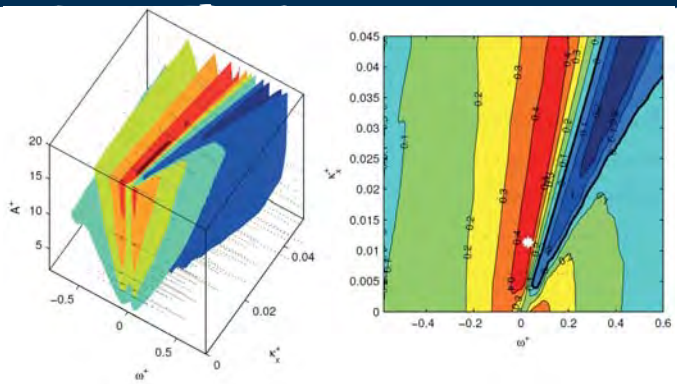
Performance of skin-friction turbulent drag reduction techniques at high Reynolds numbers

Maurizio Quadrio
PoliMI

Techniques for skin-friction turbulent drag reduction (DR) are the subject of intense research activity, owing to high applicative and practical interest. Promising active open-loop techniques have been recently identified which leverage a wall-based forcing in the spanwise direction; prominent among them are the streamwise-travelling waves (Quadrio et al, J Fluid Mech. 2009). Our knowledge of such techniques is limited to laboratory studies or Direct Numerical Simulations (DNS) where the Reynolds number Re has a very low value. On the other hand, in applications Re is typically large or very large. The current belief is that flow control performance decreases with Re: as soon as Re becomes large enough to realistically describe an application (an airplane in cruise flight, for example) the benefit would then be nearly zero.

Within the present project a massive numerical study (many thousands of DNS) has been carried out for the first time to fully characterize the streamwise-traveling waves for two values of Re in a ratio 1:5. The main outcome is that the changes with Re are not uniform in parameter space. In other words, while the relatively fast deterioration of performance of the best low-Re wave has been confirmed, other parameters have been identified to perform very well at higher Re without suffering from negative Re-effects.

The present study radically changes the perspective for technological developments of drag reduction techniques, and opens interesting fundamental questions on the physics of boundary layers at higher Re.



Parametric study of the performance of the streamwise-traveling waves in terms of percentage of skin-friction drag reduction. Traveling waves are applied to a turbulent plane channel flow studied via DNS. Left: percentage drag reduction (in color; red is 40% and blue is -20% ie drag increase) at Re=6x10^3 as a function of the 3 parameters defining the traveling wave: amplitude A+, frequency omega+ and wave number k+. Right: detailed map (at fixed A+) of the same quantity at the higher Re=3x10^4. In the two plots, every small black dot indicates where a DNS has been carried out to measure turbulent friction.

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